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**BACHELOR'S THESIS**

**STUDY OF HEAT AND MASS TRANSFER  
APPLICATIONS IN THE FIELD OF  
ENGINEERING BY USING OPENFOAM**

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## Aim

The object of this study is the development of an introductory guide on the use of the OpenFOAM software specifically oriented towards the solution of heat and mass transfer problems.

## Scope

The guide is oriented to users with a basic knowledge of fluid dynamics, heat and mass transfer and numerical methods. It has a practical approach and will teach the user throughout five chapters with a series of model problems used to develop the concepts. Each chapter includes:

- A basic description of the problem and the governing equations (intended to be a reminder about what the user is expected to be already familiar with).
- A detailed and complete description about the implementation of the case within the OpenFOAM v2.4 framework (preprocessing phase).
- Numerical resolution with OpenFOAM on a single or multiple local processors.
- A description about the main features for data extraction and analysis with a brief review of the results (post-processing phase).

This guide is limited to problems involving conduction, laminar convection and surface to surface radiation heat transfer, alone or combined. The modeling of the turbulence, radiation-participating media or phase-change are considered more advanced topics and fall outside the scope of this work, nevertheless it provides with the necessary base for developing these more advanced problems.

## Requirements

The requirements of this project are:

- Structuring the concepts in a coherent manner with increasing complexity.
- Development of the cases only within the OpenFOAM v2.4 framework.
- Brief description of the governing equations of each case.
- Descriptions about the use of the main OpenFOAM utilities for pre and post-processing.
- The proposed simulations must provide converged and consistent results.

- If possible, the simulation should be computationally light enough to be completed in a short amount of time with an average personal computer.

## Background

OpenFOAM is a free, open-source, computational fluid dynamics (CFD) software distributed by OpenCFD and the OpenFOAM Foundation under the General Public License, which gives users the freedom to modify and redistribute the software under the terms of the License.

Initially created in 1989 as a commercially licensed product named *FOAM*, it was released open-source as *OpenFOAM* in 2004. Since then it has continued receiving updates, adding functionality, and has seen an increasing adoption. Today it competes with the leading commercial softwares, such as ANSYS Fluent, and it has a large user base across most areas of engineering and science, from both commercial and academic organizations.

OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to acoustics, solid mechanics and electromagnetics. Thanks to being a full open-source product it offers a great versatility and can be customized and automatized to create individualized solutions.

Despite being open-source it has a commercial support behind from the hand of OpenCFD and CFD Direct providing software support and training courses. The current maintenance and development of the software is principally undertaken by the team of CFD Direct, with contributions from a growing community of CFD enthusiasts [14][15] [16].

## State of the art and justification

Despite being free using OpenFOAM is not necessarily cheap as the training and support costs can be important. The versatility of this software comes at the expense of a steep learning curve which is aggravated by the lack of an integrated graphic user interface (GUI) for preprocessing. And although there are several GUIs available developed by third party companies they may have their own licenses and may limit the great versatility of OpenFOAM.

Furthermore the documentation isn't abundant in general, but particularly scarce for the specific topic of heat and mass transfer, a field which also uses CFD for a wide range of applications in all the major industrial sectors, like HVAC (heating, ventilating and air-conditioning), heat exchangers, ovens, solar panels, cooling systems, etc.

An important part of the available information is based on community resources like the

*CFD Online* forums. These can be very helpful, but the information is unstructured, hard to sort and needs to be treated with special caution.

A review of the literature found some academical works as well. J. Casacuberta (2014) [6] developed a very complete and detailed guide which has strongly influenced this work and follows a similar structure but it's limited to fluid dynamics problems not involving heat transfer. A. Spinghal (2014) [8] made a brief tutorial on the use of the conjugate heat transfer solver of OpenFOAM specially detailing the structuring of the cases. M. Van Der Tempel (2012) [9] also offers a tutorial on conjugate heat transfer solving directed to more familiarized OpenFOAM users. A. Vdovin (2009) [10] provides some insight on the radiation modeling in OpenFOAM, focusing on the P1 model.

None of the previous matched the complete scope the current one pretended: with example problems of heat and mass transfer and detailed descriptions of all the steps from the generation of the mesh to the post-processing of the results.

This posed a good opportunity for this work, there certainly was a gap in information which could be a barrier for novice users, eclipsing the initial appeal the free software may have had. That's why the proposed guide is a very interesting contribution which expects to fill this gap, helping the users break through that initial barrier while saving them money in training courses, offering valuable knowledge with immediate practical applications and founding a base for a further development of the expertise in OpenFOAM.

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# Chapter 1 - Conduction

This chapter serves as a brief introduction to the OpenFOAM software while explaining the resolution of simple steady-state and transient conduction problems with `laplacianFoam`, the OpenFOAM solver for the heat equation. For more detailed information on the basics of OpenFOAM check the official user guide available at *cf.direct* [5].

## 1.1 Part A: Steady-State conduction

### 1.1.1 Description of the case

This first part of the chapter will develop an introductory case of thermal conduction through a solid concrete wall with a thermal conductivity of  $1 \text{ W/(m}\cdot\text{K)}$  and a thermal diffusivity of  $5.8 \cdot 10^{-7} \text{ m}^2/\text{s}$ . The top and bottom boundaries of the wall are adiabatic, the right face is kept at constant  $293\text{K}$  and the left has a constant inwards heat flux of  $500\text{W/m}^2$ . A diagram with the dimensions and the boundary conditions shown in Figure 1.

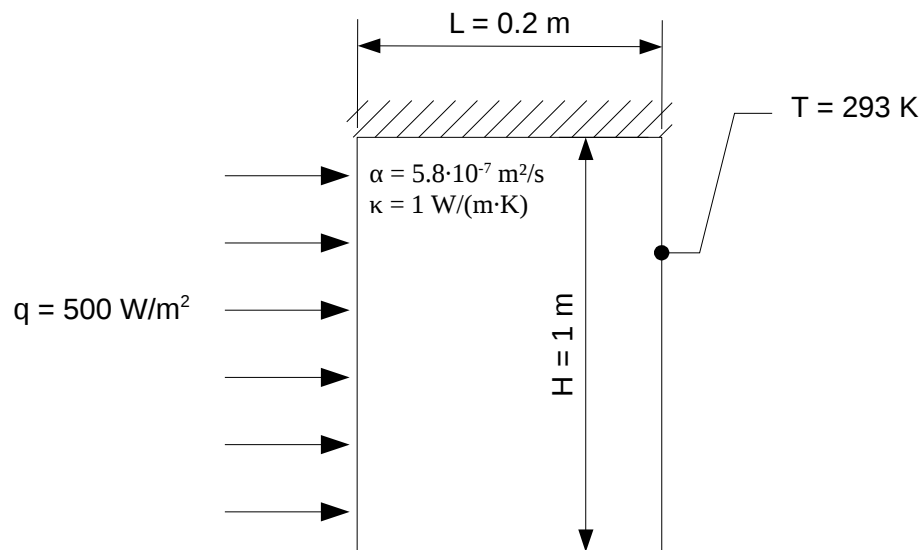


Figure 1: Diagram of the case.

#### 1.1.1.1 Assumptions

- Steady-state conditions.
- Top and bottom surfaces are adiabatic.
- Constant and uniform thermo-physical properties.
- One-dimensional heat transfer.

### 1.1.1.2 Formulation

The only mode of thermal transfer of this case is conduction and thus the distribution of heat in the wall is described by the heat diffusion equation:

$$\frac{\partial T}{\partial t} - \alpha \nabla^2 T = 0$$

Since it's a steady-state case  $\left(\frac{\partial T}{\partial t} = 0\right)$  and the heat is only transferred through the  $x$ -direction the equation is simplified as:

$$\frac{\partial^2 T}{\partial x^2} = 0$$

And therefore the general solution is:

$$T = C_1 x + C_2$$

Also, from the Fourier's Law, the heat flux in the  $x$ -direction is:

$$q_x = -\kappa \frac{\partial T}{\partial x}$$

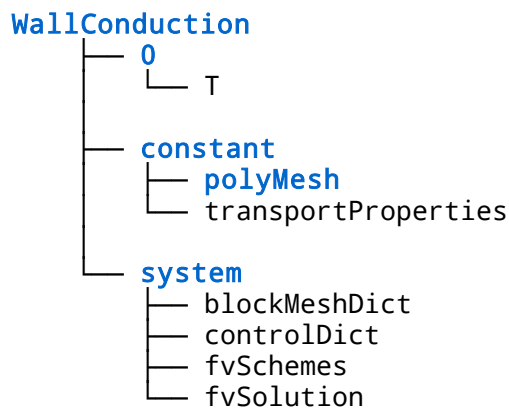
So introducing the given boundary conditions to the general solution one can easily obtain for this particular case:

$$C_1 = -500 \text{ and } C_2 = 393$$

For the resolution with OpenFOAM the solver *laplacianFoam* will be used which solves the heat equation.

### 1.1.2 Preprocessing

In OpenFOAM all the data of a simulation is stored within a user-defined case directory. The file structure for this case is shown below, the diagram includes all the data files necessary to initiate the preprocessing phase, although other files will be generated during the process.



The first step is to create the case directory (named *WallConduction* in this example) and subdirectories following the shown structure.

*Note: There must not be spaces within the case directory name and its path.*

The **constant** directory contains files specifying the physical properties of the region and a *polyMesh* folder where a full description of the mesh will be stored.

**system** contains files for setting parameters associated with the solution procedure, it can also contain dictionaries used by OpenFOAM utilities.

*Note: All the cases of this guide will use system as the default location for the blockMeshDict file, but it can also be placed inside the Polymesh folder.  
IMPORTANT: Polymesh used to be the default location and it is required in older versions of OpenFOAM.*

The **0** directory stores the initial and boundary conditions, when running the simulation more time-directories will appear containing the solution of subsequent iterations or time-steps.

This initial files are used to introduce the parameters of the simulation as the next parts will explain, they generally consist on data dictionaries, the most common mean of data input within the OpenFOAM framework. Those dictionaries contain several data entries preceded by a keyword identifying them with the general format:

```
<keyword>    <dataEntry1> <dataEntry2> ... <dataEntryN>;
```

The following steps will explain how to set up the files inside those directories. They can be created from scratch with a text editor, but one can also look for similar cases in the tutorials folder, within the OpenFOAM installation directory, in order to copy the files and edit them according to the particular simulation parameters (this case is similar to the *flange* case found in */tutorials/basic/laplacianFoam*).



### 1.1.2.1 Mesh generation

OpenFOAM always uses 3D meshes and solves the case in 3 dimensions by default. To mesh a 2D geometry a 3D mesh is created where two dimensions match the geometry and the third is arbitrary (and since the heat only transfers through the x-dimension the y-dimension is actually arbitrary for the solution of the case as well, nevertheless it will match the geometry in this example).

OpenFOAM includes a mesh generation utility named *blockMesh*, which generates meshes from a description specified in the *blockMeshDict* file. The *blockMeshDict* code for this case is the following:

```

1  /*-----* C++ *-----*\
2  | ===== |
3  | \ \ / F ield | OpenFOAM: The Open Source CFD Toolbox
4  | \ \ / O peration | Version: 2.4.0
5  | \ \ / A nd | Web: www.OpenFOAM.org
6  | \ \ / M anipulation |
7  \*-----*/
8  FoamFile
9  {
10     version      2.0;
11     format        ascii;
12     class         dictionary;
13     object        blockMeshDict;
14 }
15
16 // *****
17
18 convertToMeters 1;
19
20 vertices
21 (
22     (0 0 0) //0
23     (0.2 0 0) //1
24     (0.2 1 0) //2
25     (0 1 0) //3
26     (0 0 0.01) //4
27     (0.2 0 0.01) //5
28     (0.2 1 0.01) //6
29     (0 1 0.01) //7
30 );
31
32 blocks
33 (
34     hex (0 1 2 3 4 5 6 7) //vertex order
35     (20 1 1) //number of cells in each direction
36     simpleGrading (1 1 1) //expansion ratios
37 );
38
39 edges
40 (
41 );
42
43 boundary
44 (
45     left
46     {
47         type patch;
48         faces
49         (
50             (0 4 7 3)
51         );
52     }
53     right
54     {
55         type patch;

```

```

56         faces
57         (
58             (2 6 5 1)
59         );
60     }
61     TopBottom
62     {
63         type patch;
64         faces
65         (
66             (3 7 6 2)
67             (1 5 4 0)
68         );
69     }
70     FrontBack
71     {
72         type empty;
73         faces
74         (
75             (0 3 2 1)
76             (4 5 6 7)
77         );
78     }
79 );
80
81 // ***** //
```

The header of the file (lines 1 to 16) starts with a banner and a sub-dictionary named *FoamFile* with witch all data files that are read or written by OpenFOAM start. For the sake of clarity the header will be omitted from further code quotations.

After that follow the entries *blockMesh* will use to create the mesh:

#### **convertToMeters:**

The default unit for the coordinates are meters. This entry specifies a scaling factor by which all coordinates within *blockMeshDict* are multiplied, this way then can be expressed in other units. For example setting this to 0.01 multiplies the coordinate values by 0.01 so they are in cm.

#### **vertices:**

Here the vertices of the mesh are defined, in this case the 8 vertices of an hexahedron block. An index is assigned to each one, starting from 0, which is used to refer to those vertices in the next parts.

#### **blocks:**

This has several entries defining the mesh block and its divisions.

The array after the *hex* keyword gives the order of the vertices using their indexes to identify them. This order defines the local right-handed coordinate system of the block and follows these rules (check Figure 2 for clarification):

- The first vertex defines the origin of the local coordinate system.
- The  $x_1$  direction is described moving from the first to the second vertex.

- The  $x_2$  direction is described moving from the first to the forth.
- The first four vertices define the plane  $x_3=0$ .
- The 5<sup>th</sup>, 6<sup>th</sup>, 7<sup>th</sup> and 8<sup>th</sup> vertices are found by moving in the  $x_3$  direction from the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup> and 4<sup>th</sup> vertices respectively.

It is recommendable to already take this into account when listing the vertices. In this case they were already listed in a proper order so the order vector is (0 1 2 3 4 5 6 7).

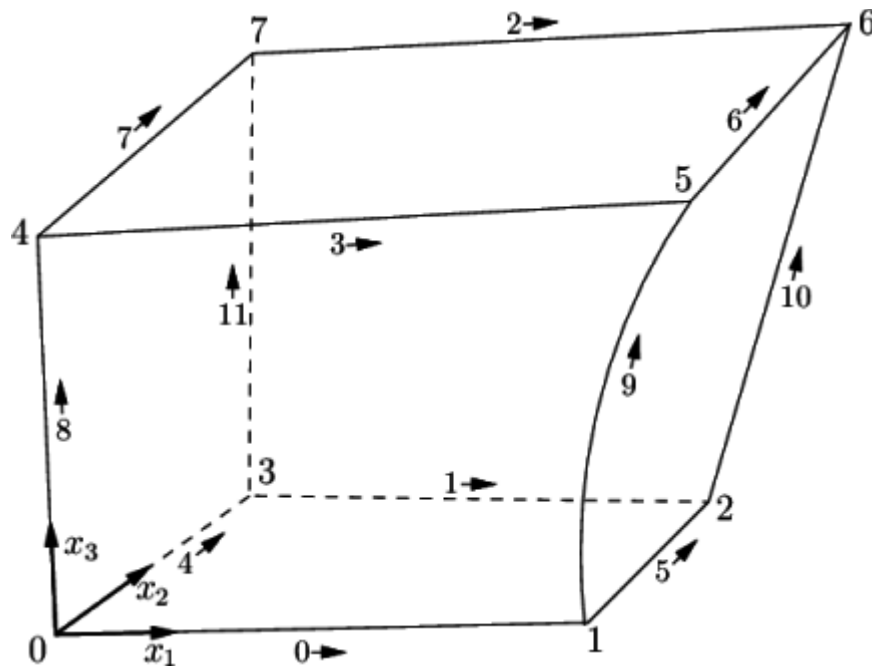


Figure 2: Diagram of a block [5]

In the second entry of **blocks** the number of divisions (cells) in each of the directions is specified. Because the heat transfer is unidimensional this case only needs divisions in the  $x$ -direction.

The third entry defines the cell expansion ratios along a direction or an edge, this is the ratio between the length of the last cell and the length of the first one. The keyword **simplegrading** is used to specify expansion ratios in the directions  $x_1$ ,  $x_2$ ,  $x_3$  defined by the local coordinate system (Figure 3 provides an example) while **edgegrading** gives the ratio along each edge according to the order and directions shown in Figure 2.

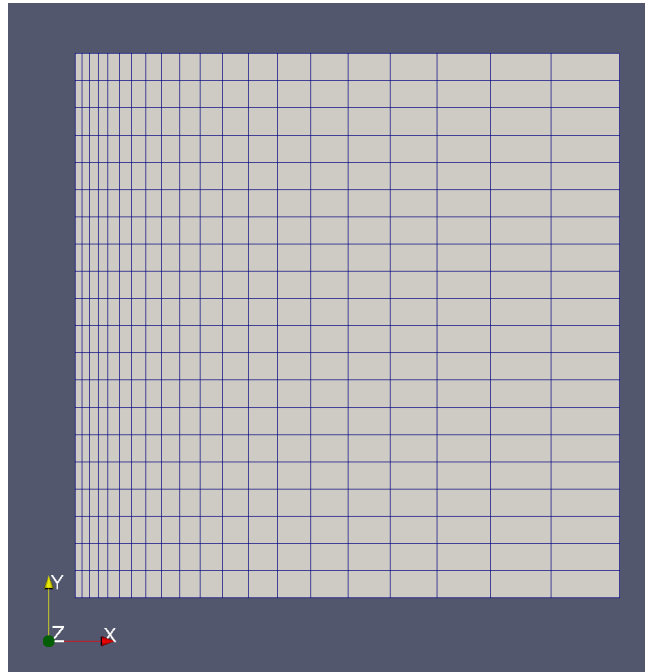


Figure 3: Example of a 20x20 mesh with a simplegrading of (10 1 1).

### edges:

It is used to describe the edges joining two vertex points (a line, an arc, a curve...). If there's no specification straight lines are assumed by default.

### boundaries:

Here the boundary of the mesh is broken into patches, regions where a boundary condition will be later applied. For this case there are four patches which have been named *left*, *right*, *TopBottom* and *FrontBack*.

After each patch name there's a *type* entry to specify its base boundary type which only describes geometrical restrictions. For the patch containing the planes normal to the z-dimension (*FrontBack*) the *empty* type is used, which instructs OpenFOAM to solve in the other two dimensions (hence this type is specific to 2D and 1D cases). The rest of patches use a generic type named *patch* which doesn't contain any geometrical information.

Finally the *faces* entry consists of one or several vectors containing the vertices of the faces assigned to the corresponding patch. Faces not specified are assigned to a *defaultFaces* patch of type *empty*.

Once the *blockMeshDict* is ready the mesh can be generated by running *blockMesh*. This is done by opening the terminal in the case directory and typing:

```
blockMesh
```

*Note: From now on, unless otherwise specified, all the described terminal commands are meant to be executed from the case directory.*

This will create all the files describing the mesh in the *Polymesh* folder. It is very recommendable to run then the *checkMesh* utility to make sure there isn't any problem with the mesh, by typing:

`checkMesh`

It's also a good idea to visualize the mesh at this point to make sure there isn't any mistake. This is done using *paraFoam*, a visual post-processing tool included in OpenFOAM. Like the previous utilities it's started by simply typing in the terminal:

`paraFoam`

This will open a *paraView* window like the one shown in Figure 4. On the *Pipeline Browser* the user can see the *WallConduction* case selected and below that a *Properties* tab. There the different mesh parts can be selected by checking the corresponding boxes. The *Volume Fields* below should have all the boxes unchecked if the boundary conditions are not set yet because it can cause errors.

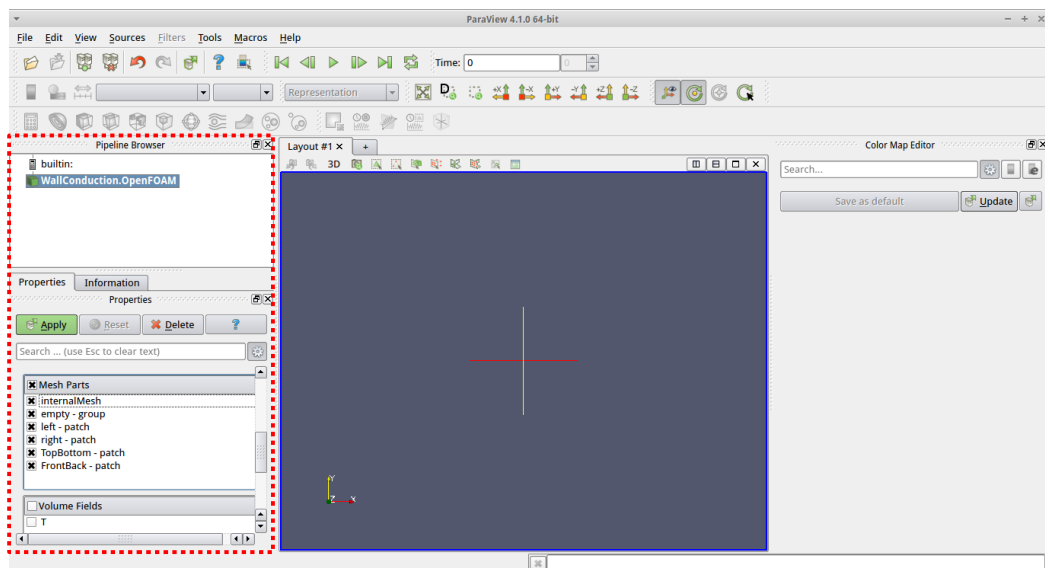


Figure 4: ParaView window. Pipeline browser and Properties marked in red.

After clicking the *Apply* button the selected parts appear in the central window. If the *Patch Names* box (within *Properties*) is selected the names of the patches will appear over the mesh, useful to make sure they are in the right faces. Also selecting *Surface with edges* or *Wireframe* at the representation pull-down menu (see Figure 5) allows the user to see the divisions of the mesh.

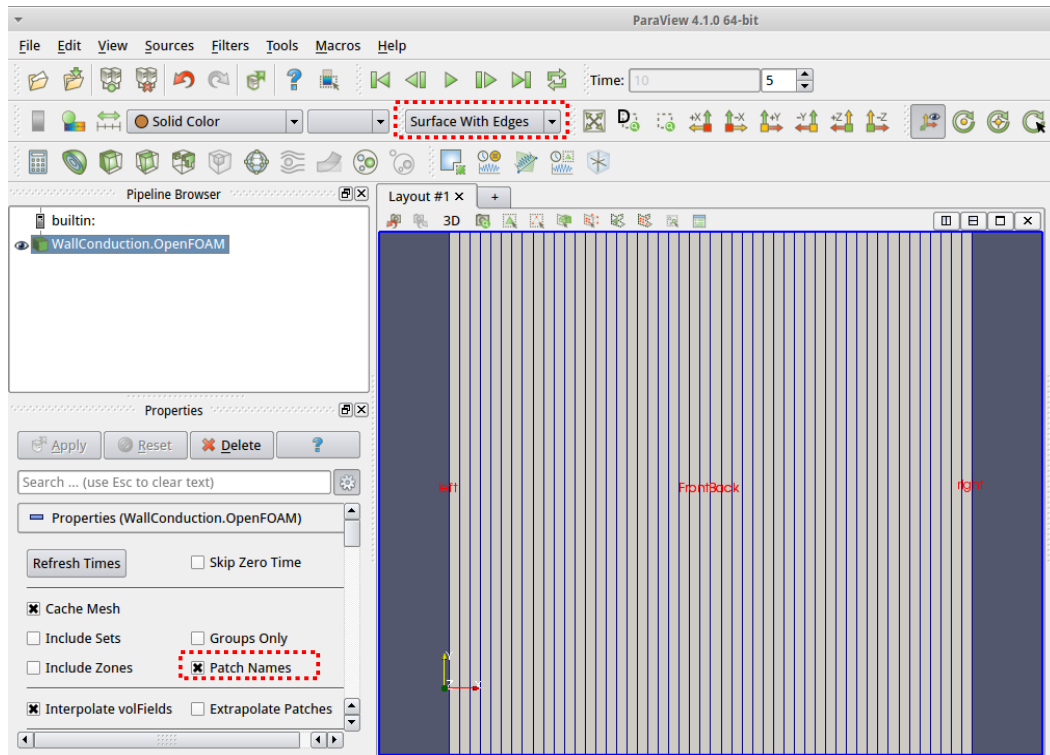


Figure 5: Viewing the mesh with paraFoam. Patch Names and representation menu marked in red.

### 1.1.2.2 Boundary and initial conditions

The next step is to establish the initial temperature field. For each field there is a corresponding file inside the *0* folder (which may be referred to *boundary file* from now on), since the only unknown of the problem is temperature there's only one file, *T*, where the initial and boundary conditions related to the temperature are introduced. For this case, it contains the following code:

```

1
2 dimensions      [0 0 0 1 0 0 0];
3
4 internalField    uniform 293;
5
6 boundaryField
7 {
8   left
9   {
10      type        fixedGradient;
11      gradient     uniform 500;
12   }
13   right
14   {
15      type        fixedValue;
16      value       uniform 293;
17   }
18   TopBottom
19   {
20      type        zeroGradient;
21   }
22 }
23

```

```

24
25     FrontBack
26     {
27         type          empty;
28     }
29 }
30
31 // *****

```

Like any other boundary file, it consists of three main entries:

#### **dimensions:**

Specifies the dimensions of the variable. The following table explains the meaning of each position:

Position	Property
1	Mass
2	Length
3	Time
4	Temperature
5	Quantity of substance
6	Current
7	Luminous intensity

Table 1: Properties corresponding to each position of the dimensions entry.

OpenFOAM works with SI units by default. The number at each position within the array indicates the corresponding exponent, e.g. [1 3 0 0 0 0 0] would be used to express  $\text{Kg/m}^3$ .

Since this file corresponds to the temperature variable the entry is set correspondingly to [0 0 0 1 0 0 0].

#### **internalField:**

In this entry the initial internal field is defined. `uniform` sets the specified value (293) to all the internal elements. For steady-state cases this doesn't affect the final solution but may have an impact on the stability and resolution speed.

#### **boundaryField:**

Establishes the boundary conditions at each of the patches defined in the *Mesh generation* section:

- *left*: a `fixedGradient` type is used which specifies the normal gradient

$\left(-\frac{\partial T}{\partial x}\right)$ , this way the fixed thermal flux condition can be established

remembering that:  $-\frac{\partial T}{\partial x} = \frac{q}{k}$ .

- *right*: The fixed temperature condition is directly specified with the `fixedValue` type.
- *TopBottom*: `zeroGradient` sets the normal gradient ( $\pm \frac{\partial T}{\partial y}$ ) to 0, establishing this way the adiabatic condition.
- *FrontBack*: Like in `blockMeshDict`, the empty type needs to be specified here as well.

### 1.1.2.3 Physical properties

The only physical property OpenFOAM needs for this case is the thermal diffusivity of the material (the parameter  $\alpha$  from the heat equation), which is defined within `transportProperties` where is named `DT`.

```
1
2  DT      DT [ 0 2 -1 0 0 0 ] 5.8e-07; //Concrete
3
4
5  // ***** //
```

### 1.1.2.4 Time and I/O settings

The parameters related to the control of the time of the simulation and the input/output of the data are introduced in the `controlDict` dictionary. In the case of steady-state simulations like this the time controls relate to the number of iterations. The used code is the following:

```
1  application      laplacianFoam;
2
3  startFrom        latestTime;
4
5  startTime        0;
6
7  stopAt           endTime;
8
9  endTime          10;
10
11 deltaT           1;
12
13 writeControl      timestep;
14
15 writeInterval     2;
16
17 purgeWrite        0;
18
19 writeFormat       ascii;
20
21 writePrecision    6;
22
```



```

23 writeCompression off;
24
25 timeFormat      general;
26
27 timePrecision   6;
28
29 runTimeModifiable true;
30
31
32 // *****

```

Some of the more relevant entries are:

- **startFrom:** Controls the start time of the simulation. **latestTime** instructs the solver to begin from the latest stored time-folder, this is useful to resume simulations. The keyword **startTime** can be used to tell it to start from the time specified at the **startTime** entry which otherwise has no use.
- **stopAt:** Controls the ending of the simulation, in this case the value specified at the **endTime** entry.
- **deltaT:** Specifies the time-step. In steady-state problems every time step is an iteration.
- **writeControl:** Controls the timing of the write output file. With **timestep** it writes every **writeInterval** time-steps and with **runtime** every **writeInterval** simulated seconds.
- **purgewrite:** Specifies a limit on the number of output time-directories stored, upon reaching the limit the latest output will overwrite the oldest one. 0 is for no limit.

### 1.1.2.5 Discretization and linear solver settings

The finite volume discretization schemes are specified in *fvSchemes*, and *fvSolution* is used for the specification of the linear equation solvers and tolerances and other algorithm controls.

*fvSchemes:*

```

1 ddtSchemes
2 {
3     default          steadyState;
4 }
5
6 gradSchemes
7 {
8     default          Gauss linear;
9     grad(T)          Gauss linear;
10 }
11
12 divSchemes
13 {
14     default          none;

```

```

15 }
16
17 laplacianSchemes
18 {
19     default          none;
20     laplacian(DT,T) Gauss linear corrected;
21 }
22
23 interpolationSchemes
24 {
25     default          linear;
26 }
27
28 snGradSchemes
29 {
30     default          corrected;
31 }
32
33 fluxRequired
34 {
35     default          no;
36     T                ;
37 }
38
39
40 // ***** //

```

*fvSolution:*

```

1  solvers
2  {
3      T
4      {
5          solver          PCG;
6          preconditioner  DIC;
7          tolerance       1e-6;
8          relTol          0;
9      }
10 }
11
12 SIMPLE
13 {
14     nNonOrthogonalCorrectors 0;
15 }
16
17
18 // ***** //

```

This guide won't go into details about those, the only highlight is the `ddtScheme` within `fvSchemes` which needs to be set to `steadyState` for the steady-state resolution.

### 1.1.3 Running the simulation

To run the `laplacianFoam` solver from the foreground, like with the utilities the corresponding command is typed in the terminal:

```
laplacianFoam
```

During the execution the terminal outputs the time being resolved (in this case it corresponds to the iteration as already explained) and the initial and final residuals. This output can be logged to a file by using this command instead:

```
laplacianFoam | tee [filename]
```

And yet another option is (if the screen argument isn't used it runs on the background):

```
foamJob -screen laplacianFoam
```

As soon as the first results are written to time-folders they are ready to be post-processed, and after the 10 specified iterations the execution of the solver stops. The residuals should be very low which can be an indicator the solution is well converged, in fact this case converges at the first step.

### 1.1.4 Post-processing

This section will cover the visualization of the results using *paraFoam*. The first steps are similar as the ones carried at 1.1.2.1 to view the mesh: once the application is loaded the mesh parts the user wants to visualize are selected on the *Properties* menu, and this time the *T* field, within *Volume Fields*, needs to be checked as well, then click on Apply.

Now *paraFoam* is ready to display the results. Figure 6 marks some of the controls which will be used on the following steps.

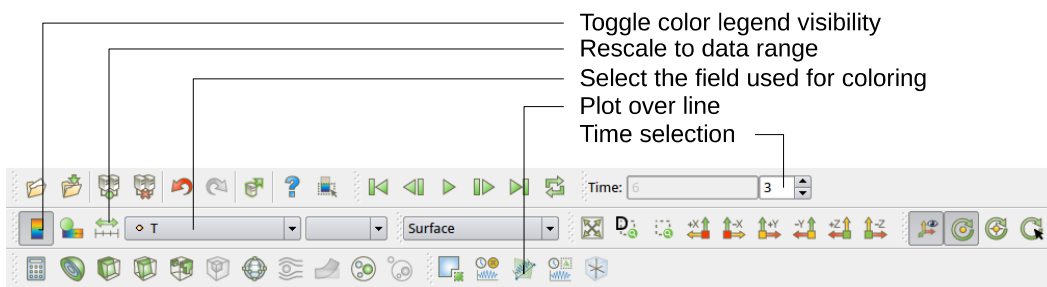


Figure 6: Some basic post-processing controls.

The *Surface* representation should be selected. Around the top left of the interface there's a box where the user can select which field *paraFoam* is using to generate the color map on the mesh (*Solid Color* will be selected as default). There are two entries for *T*, the one with a cube icon uses the solved value of *T* at each cell and the one with a point interpolates the values across the cells resulting in a smoother appearance. There's also a control to toggle a legend for the color map as shown in the figure.

The *Time* selection box allows the user to navigate through the stored results at the time-folders. When doing so, the data range between different times may change so the *Rescale to data range* option should be used.

There are different color presets for the color mapping which can be chosen by clicking on the icon with the folder and a heart to the right, within the *Color Map Editor*.

*paraFoam* can also generate graphs for the temperature distribution across an user

defined path through the mesh. This is done by clicking on the *Plot over line* filter<sup>1</sup>, then on the *Properties* menu the user can define a path line through two points or choose an axis. After clicking *Apply* a new window opens with the graph and the *Properties* menu is extended with some more options, among them a *Line Series* sub-menu where the fields of interest can be toggled (in case was were more than one).

Figure 7 shows the obtained results for the last iteration ( $t=10$ ). It's a line crossing the vertical axis at  $T=393K$  and with a slope of  $-500K/m$ , therefore matching the analytical solution:

$$T = -500x + 393.$$

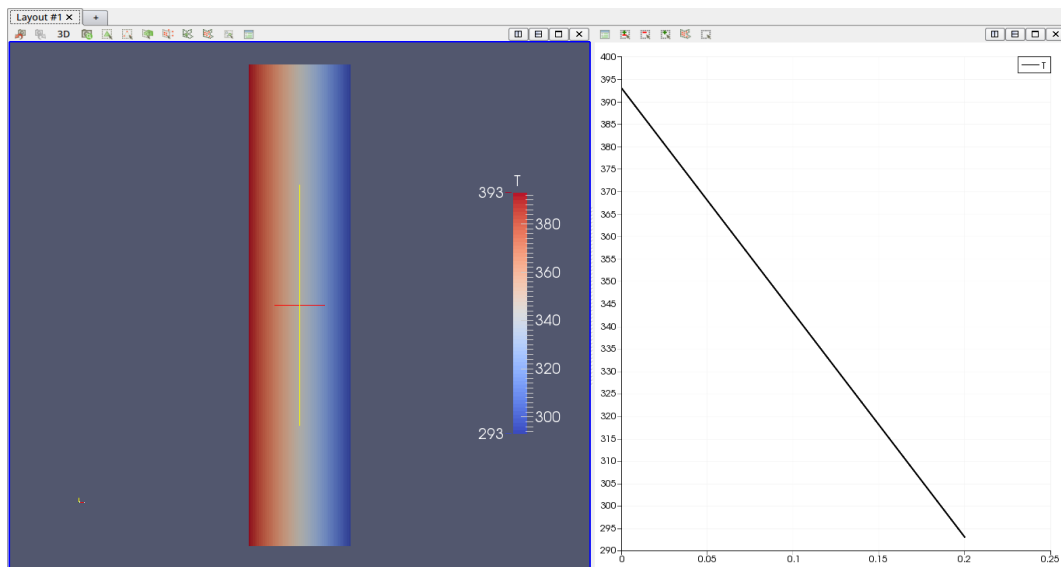


Figure 7: Obtained results at  $t=10$ . Left: color map of the temperatures. Right: Temperature over the X axis.

<sup>1</sup> paraFoam has different tools to help extracting and processing the desired data named filters.

## 1.2 Part B: Transient conduction

### 1.2.1 Description of the case

This case maintains the dimensions, properties and boundaries of the previous one, except for the right boundary which now has a time dependent temperature condition and therefore its a transient problem. This new condition is described by:

$$T_{\text{right}} = 293 + 20 \cdot \sin(2\pi f \cdot t) \quad \text{With } f = \frac{1}{86400}$$

Which corresponds to a sinusoidal oscillation of 20K around 293K and with a period of 86400s (one day).

The initial condition is the steady-state solution at  $t = 0$  (the solution of the previous case).

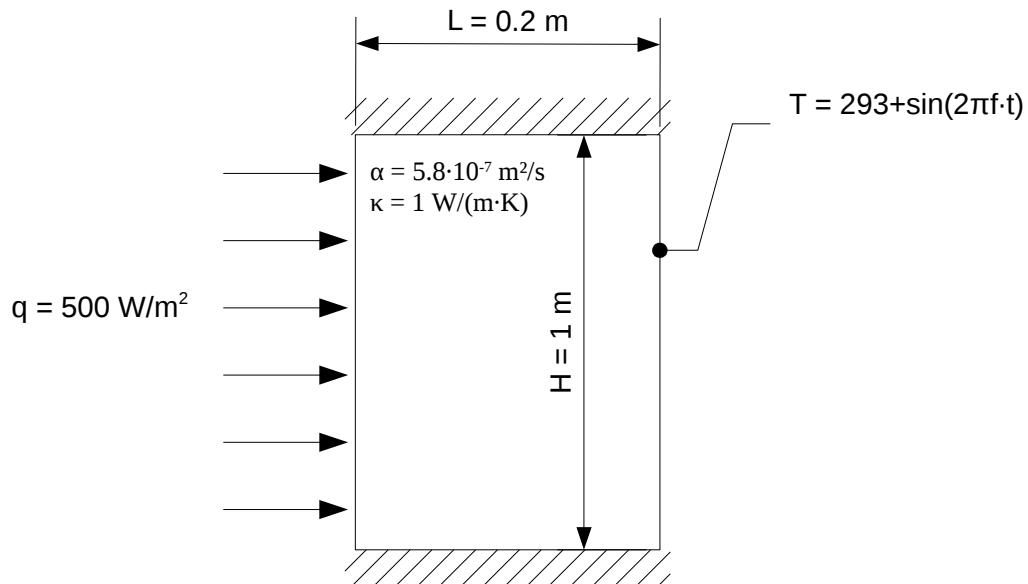


Figure 8: schematic of the new problem

#### 1.2.1.1 Assumptions

- Top and bottom surfaces are adiabatic.
- Constant, uniform thermo-physical properties.
- One-dimensional conduction.

#### 1.2.1.2 Formulation

Like in the previous case the governing equation is the heat equation but now the temporal term isn't null:

$$\frac{\partial T}{\partial t} - \alpha \nabla^2 T = 0$$

Consequently the case can still be handled with the `laplacianFoam` solver.

## 1.2.2 Preprocessing

This case will be treated as a modification of the previous one. The mesh is kept the same so the *Polymesh* contents can be reused, and the rest of files only have minor modifications.

### 1.2.2.1 Boundary and initial conditions

In order to use the solution of the previous case as the initial condition of this one it's enough to copy the *T* file from the last time-folder and place it in the *0* folder of this case. The user can observe now the internal field is a list of the calculated values for each cell and below there's the `boundaryField` sub-dictionary with the previous specification of the boundary. Next is necessary to edit this to include the new boundary condition:

*Note: To use the fields from a previous solution without special modifications the mesh must remain the same.*

```

1  boundaryField
2  {
3      left
4      {
5          type          fixedGradient;
6          gradient      uniform 500;
7      }
8      right
9      {
10         type          oscillatingFixedValue;
11         refValue      uniform 1;    // Reference value for oscillation
12         offset        292;         // Oscillation mean value offset
13         amplitude      constant 20; // Amplitude of oscillation
14         frequency      constant 1.1574e-5; // frequency (1/86400)
15     }
16     TopBottom
17     {
18         type          zeroGradient;
19     }
20     FrontBack
21     {
22         type          empty;
23     }
24 }
```

The right face of the wall (`right` patch) now has a condition of the type `oscillatingFixedValue` which is used to specify a condition of the kind:

$$refValue \cdot (1 + amplitude \cdot \sin(2\pi \cdot frequency \cdot t)) + offset$$

Thus:

$$T_{\text{right}} = 1 \cdot \left(1 + 20 \cdot \sin\left(\frac{2\pi t}{86400}\right)\right) + 292 = 293 + 20 \cdot \sin\left(\frac{2\pi t}{86400}\right)$$

### 1.2.2.2 Control and schemes

Finally the *controlDict* and *fvSchemes* dictionaries also need some modifications.

In *fvSchemes* a transient scheme has to be specified within *ddtSchemes*. For this example the Crank-Nicolson scheme is used. Next to the corresponding keyword there's an off-centering coefficient which can weight the scheme from a pure implicit Euler method (0) to pure Crank-Nicolson (1).

```

1 ddtSchemes
2 {
3     default          CrankNicolson 1;
4 }
5
```

In *controlDict* some time parameters are modified to set a simulation time of two days with a time-step of 360 seconds (which relative to the speed of the problem is small enough to provide good time precision) and a write interval of an hour:

```

1 application      laplacianFoam;
2
3 startFrom        startTime;
4
5 startTime        0;
6
7 stopAt           endTime;
8
9 endTime          172800;
10
11 deltaT           360;
12
13 writeControl      runtime;
14
15 writeInterval     3600;
16
17 purgeWrite       0;
18
19 writeFormat       ascii;
20
21 writePrecision    6;
22
23 writeCompression off;
24
25 timeFormat        general;
26
27 timePrecision     6;
28
29 runtimeModifiable true;
```

### 1.2.3 Post-processing

After running `laplacianFoam` the results can be evaluated in the same way as the precious problem. Since now the solution has a time dependence, with `paraFoam` the user can navigate through the written results (every 3600s) to check the temperature distribution at the given time, but the application has also some functions to plot data over time which will be introduced next (see Figure 10 for a reference on the controls).

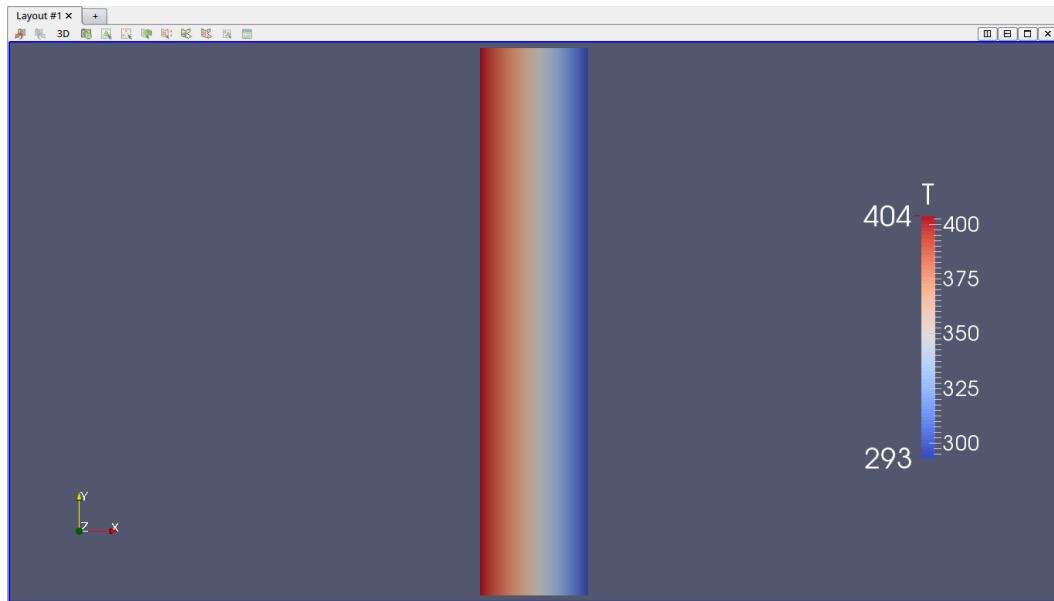


Figure 9: Temperature distribution at  $t=43200s$  (12h)

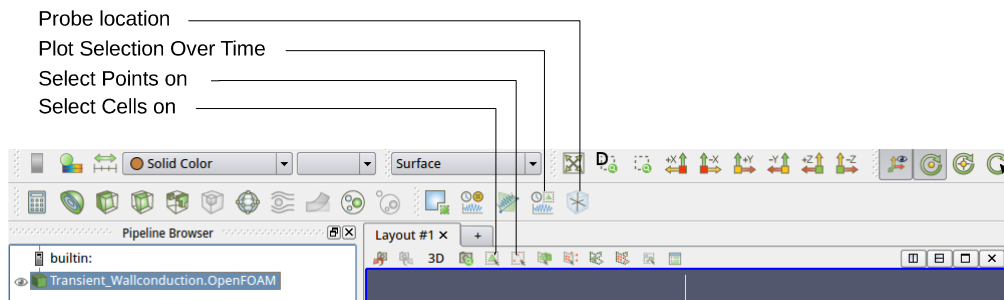


Figure 10: Reference for the described controls to plot the fields at a desired location.

One way to plot the results over time is to directly select a cell on the 3D view with *Select Cells on* (the selected cell will appear with a purple outline) and then click on *Plot Selection Over Time* and *Apply*; a new window will appear with the corresponding chart (the desired fields can be selected on the *Properties* menu). For example Figure 11 shows the result for the right face, which naturally is the imposed boundary condition.



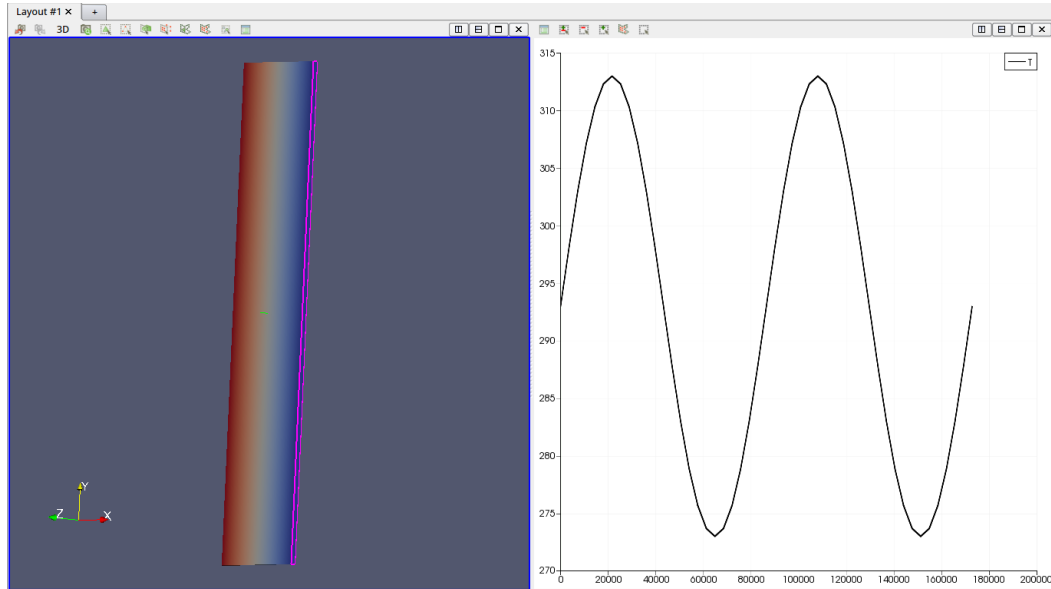


Figure 11: At left the selected face and at right the corresponding temperature-time chart.

There's also the possibility to plot the fields at a given coordinate. To do so first the user has to click on *Probe Location* and, on the *Properties* menu, insert the coordinates of the point and then click *Apply*. In the *Pipeline Browser* only the eye icon next to *ProbeLocation* should be highlighted so it's the only element displayed in the 3D view, this way the user can then click on *Select Points on* and drag a rectangle to select the point (the point appears as a purple dot when selected). After that the user only has to use *Plot Selection Over Time* again to generate the graph.

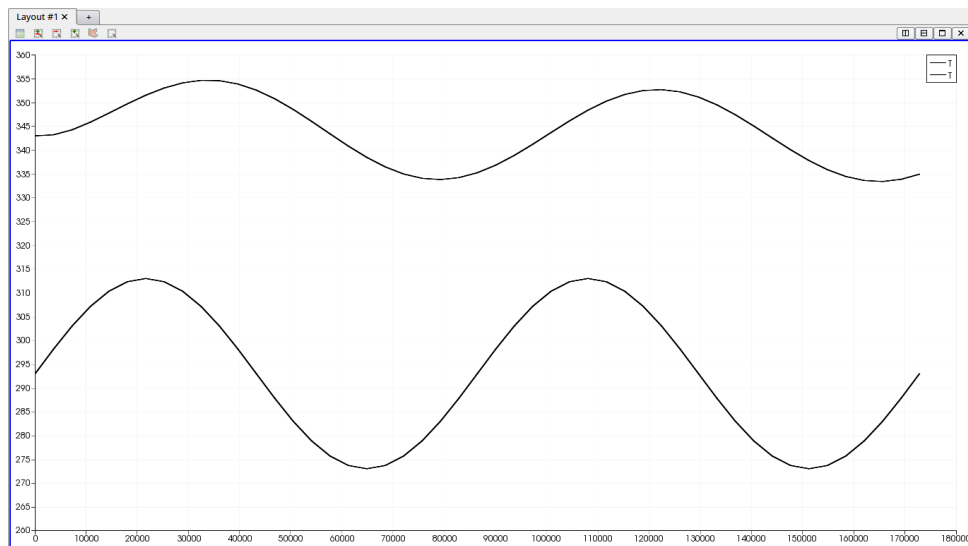


Figure 12: Chart of the temperature at the right face (down) and at the center of the wall (up).

Finally some comments about the displaying controls. On the top right of the central window there are some buttons to close it or split it, this creates an “empty” window with

a list of options. When having this empty window selected the eye icons on the *Pipeline Browser* can be used to control what is displayed, be it a chart or a 3D entity. In a similar way multiple graphs can be displayed at once (like in Figure 12) by having the chart window selected and using the corresponding eye icons.

# Chapter 2 - Multiple Materials

This chapter introduces the `chtMultiRegionSimpleFoam` (*chtMRSF*) solver for the resolution of steady-state conduction problems involving different materials. This solver uses a particular case structure which will be detailed here. `chtMultiRegionSimpleFoam` also allows the solution of conjugate heat transfer problems (problems combining conduction and convection) which will be explained in *Chapter 4*.

## 2.1 Description of the case

The model case consists on a 2D block formed by three different materials. The bottom of the block is adiabatic, the top receives a constant inwards heat flux and each side is exposed to a fluid with a known, constant, uniform temperature and heat transfer coefficient. Figure 13 summarizes these boundary conditions and the geometry and the thermal conductivity of each material is indicated in Table 2.

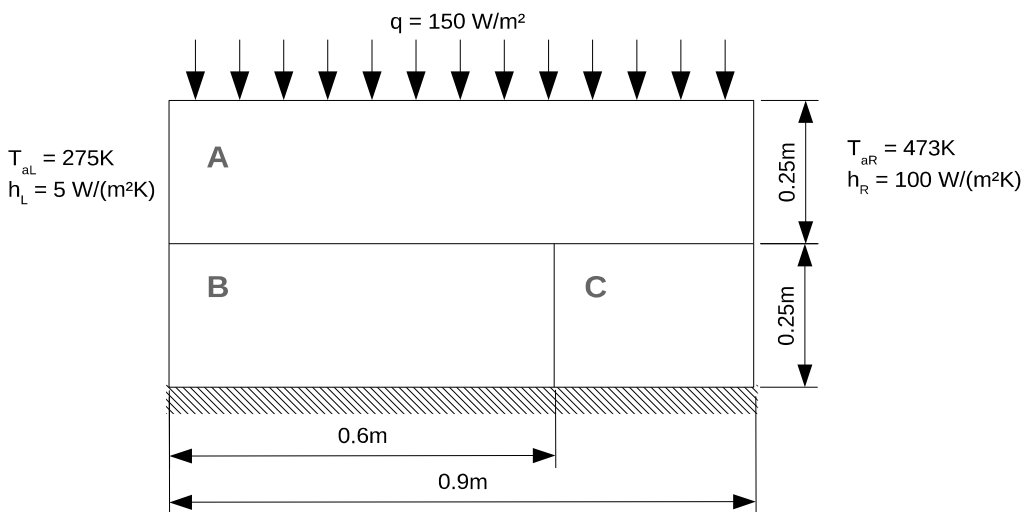


Figure 13: Schematic of the case.

Material	Thermal conductivity [W/(m² · K)]
A	0.5
B	210
C	2

Table 2: Thermal conductivities of the materials.

### 2.1.1 Assumptions

- Bi-dimensional heat transfer
- Steady-state conditions
- Constant, uniform thermo-physical properties
- No contact resistance between materials
- Known heat transfer coefficients
- Negligible radiation exchange with surroundings.

### 2.1.2 Formulation

Like the previous chapter this is a conduction problem described by the heat equation and the Fourier's Law, which with the proper simplifications are reduced to:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

$$\vec{q} = -\kappa \left( \frac{\partial T}{\partial x} \vec{i} + \frac{\partial T}{\partial y} \vec{j} \right)$$

As for the convection heat transfer at the side walls, it is modeled according to the Newton's law of cooling:

$$q_{\text{out}} = h(T_{\text{wall}} - T_a)$$

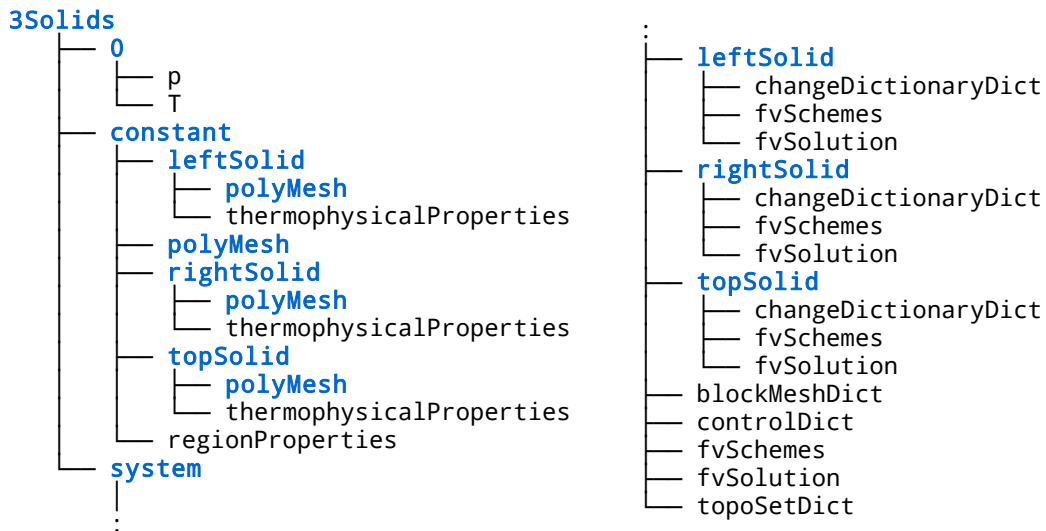
But note that since the heat transfer coefficients (h) are assumed known this case isn't really dealing with the convection problem (this will be done in the next chapter).

## 2.2 Preprocessing

Despite this case being very similar to the one in the first chapter its structure is quite different because now there are three different regions, one for each material. The `laplacianFoam` solver can't handle multiple regions without modifying the code, so this problem will be solved with `chtMultiRegionSimpleFoam`, a steady-state solver which can deal with processes involving heat transfer between different solids and between a solid and a fluid (but again, the convection problem isn't resolved yet in this chapter).

*Note: The transient version of `chtMultiRegionSimpleFoam` is `chtMultiRegionFoam` and it follows the same structure. “cht solvers” may be used to refer to both.*

The diagram below shows the new file structure of the case. The main difference with the previous is that now there's a specific folder for every material, both in the *constant* and *system* directories. These folders contain information or dictionaries specific to each region and can be named however the user prefers to identify each region (remembering that there should be no spaces). For this example they are *leftSolid* (material B), *rightSolid* (material C) and *topSolid* (material A).



## 2.2.1 Mesh Generation

The meshing strategy is to create a single 2D mesh for the whole domain and then (after specifying the boundary conditions) use the *splitMeshRegions* tool to divide it in the three different regions. The mesh is generated using *blockMesh* with the following *blockMeshDict* code:

```

1  convertToMeters 1;
2
3  vertices
4  (
5      (0 0 -0.01)
6      (0.9 0 -0.01)
7      (0.9 0.5 -0.01)
8      (0 0.5 -0.01)
9      (0 0 0.01)
10     (0.9 0 0.01)
11     (0.9 0.5 0.01)
12     (0 0.5 0.01)
13 );
14
15 blocks
16 (
17     hex (0 1 2 3 4 5 6 7) (90 50 1) simpleGrading (1 1 1)
18 );
19
20 edges
21 (
22 );
23
24 boundary
25 (
26     maxY
27     {
    
```

```

28         type wall;
29         faces
30         (
31             (3 7 6 2)
32         );
33     }
34     minX
35     {
36         type wall;
37         faces
38         (
39             (0 4 7 3)
40         );
41     }
42     maxX
43     {
44         type wall;
45         faces
46         (
47             (2 6 5 1)
48         );
49     }
50     minY
51     {
52         type wall;
53         faces
54         (
55             (1 5 4 0)
56         );
57     }
58 );
59 );
60
61 mergePatchPairs
62 (
63 );
64
65 // ***** //
```

Although the boundary faces could be a `patch` type, with the `wall` type the heat rates across them can be quickly obtained with a built-in post-processing tool later. The front and back faces (z-axis) are undefined so they are automatically assigned to the `defaultFaces` group with an empty type.

### 2.2.2 Initial and boundary conditions

The boundary conditions are initially specified in the `T` file inside the `0` directory. Also there has to be `p` file because it is required by the `thermophysicalProperties` dictionary although it doesn't have any physical meaning in this case.

`T`:

```

1  dimensions      [0 0 0 1 0 0 0];
2
3  internalField    uniform 300;
4
5  boundaryField
6  {
7      maxY
8      {
9          type      externalWallHeatFluxTemperature;
10         kappa      solidThermo;
11         q           uniform 150;
```

```

12         value          uniform 300.0;
13         kappaName      none;
14     }
15     minY
16     {
17         type            zeroGradient;
18     }
19     minX
20     {
21         type            externalWallHeatFluxTemperature;
22         kappa           solidThermo;
23         Ta              uniform 275;
24         h              uniform 5;
25         value          uniform 300.0;
26         kappaName      none;
27     }
28     maxX
29     {
30         type            externalWallHeatFluxTemperature;
31         kappa           solidThermo;
32         Ta              uniform 473;
33         h              uniform 100;
34         value          uniform 300.0;
35         kappaName      none;
36     }
37
38     defaultFaces
39     {
40         type            empty;
41     }
42 }
43
44
45 // ***** //
```

*p*:

```

1  dimensions      [1 -1 -2 0 0 0 0];
2
3  internalField   uniform 1e5;
4
5  boundaryField
6  {
7      ".*"
8      {
9          type      calculated;
10     }
11 }
```

The `externalWallHeatFluxTemperature` type used in *T* can impose a fixed heat flux condition by directly specifying it (`q` keyword, positive value for entering flux) or a fixed heat transfer coefficient condition (i.e.  $q_{\text{out}} = h(T_{\text{wall}} - T_a)$ ) introducing the heat transfer coefficient (`h`) and the ambient temperature (`Ta`) instead. Also this condition obtains the thermal conductivity from the properties specified for each region and it only needs to be told it's a solid material with `solidThermo` next to the `kappa` keyword. The `value` entry is just the initial temperature value.

As for *p*, all patches (`".*"`)<sup>2</sup> are simply given a `calculated` type.

<sup>2</sup> The `".*"` is a "wildcard" character (i.e. it stands for any character) that can be used to apply a condition to any patch (`".*"`), any patch whose name begins with certain string (`"string.*"`), etc.

### 2.2.3 Mesh splitting

In order to split the mesh with the *splitMeshRegions* tool the different regions of the mesh have to be defined with the *topoSet* tool using the following *topoSetDict* dictionary:

```

1  actions
2  (
3
4      // leftSolid
5      {
6          name    leftSolid; //name of the set
7          type    cellSet;
8          action  new; //create a new set
9          source  boxToCell; //use a selection box
10         sourceInfo
11         {
12             box (0 0 -1 )(0.6 0.25 1); //box corners
13         }
14     }
15     {
16         name    leftSolid;
17         type    cellZoneSet;
18         action  new;
19         source  setToCellZone;
20         sourceInfo
21         {
22             set leftSolid;
23         }
24     }
25
26     // rightSolid
27     {
28         name    rightSolid;
29         type    cellSet;
30         action  new;
31         source  boxToCell;
32         sourceInfo
33         {
34             box (0.6 0 -1 )(0.9 0.25 1);
35         }
36     }
37     {
38         name    rightSolid;
39         type    cellZoneSet;
40         action  new;
41         source  setToCellZone;
42         sourceInfo
43         {
44             set rightSolid;
45         }
46     }
47
48     // topSolid
49     {
50         name    topSolid;
51         type    cellSet;
52         action  new;
53         source  boxToCell;
54         sourceInfo
55         {
56             box (0 0.25 -1 )(0.9 0.5 1);
57         }
58     }
59     {
60         name    topSolid;
61         type    cellZoneSet;
62         action  new;
63         source  setToCellZone;
64         sourceInfo
65         {
66             set topSolid;

```



```

67     }
68   }
69 );
70
71 // ***** //

```

The definition has two parts, the first one (lines 5 to 14) creates a `cellSet` using a selection box which is defined by the coordinates of the two opposed corners, the box doesn't need to match the domain as long as it contains only the desired part of the mesh. Next (lines 15 to 24) a `cellZone` is created by using the previous `cellSet` as a source. This is repeated for each region. With this `topoSet` will extract and store the necessary information to divide the mesh into the corresponding regions after executing it by typing in the terminal:

```
topoSet
```

After that typing:

```
splitMeshRegions -cellZones -overwrite
```

Will execute the *splitMeshRegions* tool which will divide the mesh according to the specified `cellZones` and store the split meshes within the corresponding region-folder, inside constant.

To view this divided meshes first is necessary to use the next command to prepare the `.OpenFOAM` file of each region:

```
paraFoam -touchAll
```

And next the user can launch *paraview* to open them:

```
paraview
```

The regions are opened by clicking on *Open*, in the *File* menu, and selecting the corresponding `.OpenFOAM` files. Multiple files can be selected to open them at once. After that each region will appear in the pipeline browser and can be handled separately.

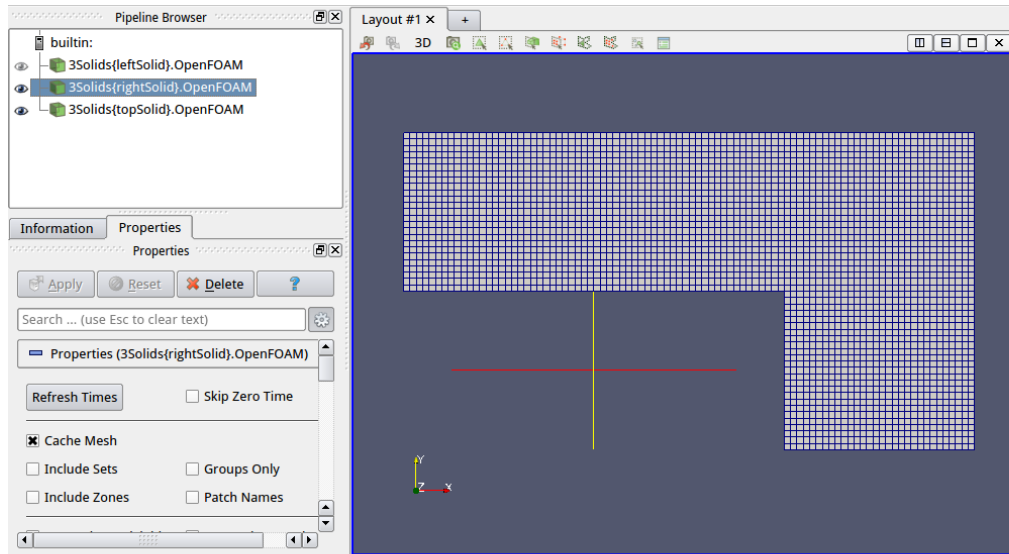


Figure 14: Visualization of the *topSolid* and *rightSolid* internal meshes.

*splitMeshRegions* will also create three new folders inside the *0* directory with their own *T* and *p* files, the ones the solver will actually use. These new *T* and *p* files are based on those defined in 2.2.2 so the external faces already have the proper condition, but the internal faces are given a default calculated type which, for *T*, has to be changed to `compressible::turbulentTemperatureCoupledBaffleMixed`, a special type for coupling the different regions.

So, for example, the *T* file of the *leftSolid* has this part:

```

1     leftSolid_to_rightSolid
2     {
3         type            calculated;
4         value            uniform 0;
5     }
6     leftSolid_to_topSolid
7     {
8         type            calculated;
9         value            uniform 0;
10    }
```

Which has to be changed to:

```

1     leftSolid_to_rightSolid
2     {
3         type            compressible::turbulentTemperatureCoupledBaffleMixed;
4         Tnbr            T;
5         kappa            solidThermo;
6         kappaName        none;
7         value            uniform 300;
8     }
9     leftSolid_to_topSolid
10    {
11         type            compressible::turbulentTemperatureCoupledBaffleMixed;
12         Tnbr            T;
13         kappa            solidThermo;
14         kappaName        none;
15         value            uniform 300;
16    }
```

The same is repeated for the other regions.

There's a specific tool to replace entries and automatize this process, the *changeDictionary*. It uses the *changeDictionaryDict* located in the corresponding region-folder in *system*. For the *leftSolid* this dictionary should be:

```

1 dictionaryReplacement
2 {
3     T
4     {
5         boundaryField
6         {
7             "leftSolid_to.*"
8             {
9                 type
compressible::turbulentTemperatureCoupledBaffleMixed;
10                 Tnbr T;
11                 kappa solidThermo;
12                 kappaName none;
13                 value uniform 300;
14             }
15         }
16     }
17 }
18
19 // ***** //
```

With this, after executing in the terminal:

```
changeDictionary -region leftSolid
```

The entries from the patches of the *T* file of the *leftSolid* whose name starts with "leftSolid\_to" will be replaced by the ones in the *changeDictionaryDict*.

It's possible to go further and make an script by creating a new text file (e.g. *changeT*) in the case directory with:

```

1 #!/bin/sh
2
3 for i in leftSolid rightSolid topSolid
4 do
5     changeDictionary -region $i
6 done
```

This way the *changeDictionary* of each region can be executed by simply launching the file from the terminal:

```
bash changeT
```

## 2.2.4 Physical properties

The *chtMRSF* solver relies on the *thermophysicalProperties* dictionary which establishes the material properties and the thermo-physical model.

The first part is common on the three regions, it sets a model for a solid material with constant properties:

```

1 thermoType
2 {
3     type            heSolidThermo;
4     mixture         pureMixture;
5     transport       constIso;
6     thermo          hConst;
7     equationOfState rhoConst;
8     specie          specie;
9     energy          sensibleEnthalpy;
10 }

```

The second part defines the thermal conductivity ( $\kappa$ ) of each material among other unnecessary properties which are just placeholders, as they aren't relevant for the governing equations of the case. E.g. for the *leftSolid*:

```

11 mixture
12 {
13     specie
14     {
15         nMoles      1;
16         molWeight   12;
17     }
18     transport
19     {
20         kappa       210;
21     }
22     thermodynamics
23     {
24         Hf          0;
25         Cp          450;
26     }
27     equationOfState
28     {
29         rho         8000;
30     }
31 }
32 }
33 }
34 }

```

Also within the constant directory there is a file named *regionProperties* which indicates the solver the names of the *solid* and *fluid* regions to solve, both entries must be present but as there aren't fluid regions this one is left void:

```

1 regions
2 (
3     fluid      ()
4     solid      (leftSolid rightSolid topSolid)
5 );
6
7 // *****

```

## 2.2.5 Control, solution and schemes

The three regions use the same *fvSchemes* and *fvSolution* inside the corresponding region folder in *system*.

*system/regionFolder/fvSchemes:*

```

1  ddtSchemes
2  {
3      default          steadyState;
4  }
5
6  gradSchemes
7  {
8      default          Gauss linear;
9  }
10
11 divSchemes
12 {
13     default          none;
14 }
15
16 laplacianSchemes
17 {
18     default          none;
19     laplacian(alpha,h) Gauss linear uncorrected;
20 }
21
22 interpolationSchemes
23 {
24     default          linear;
25 }
26
27 snGradSchemes
28 {
29     default          uncorrected;
30 }
31
32 fluxRequired
33 {
34     default          no;
35 }
36
37 // ***** //
```

*system/regionFolder/fvSolution:*

```

1  solvers
2  {
3      h
4      {
5          solver          PCG;
6          preconditioner  DIC;
7          tolerance       1e-06;
8          relTol          0;
9      }
10 }
11
12 SIMPLE
13 {
14     nNonOrthogonalCorrectors 0;
15 }
16
17
18 // ***** //
```

Also to prevent errors the *fvSolution* and *fvSchemes* in the *system* directory are left there, but they contain no information besides the header.

*system/fvSolution:*

```

1 FoamFile
2 {
3     version      2.0;
4     format       ascii;
5     class        dictionary;
6     object       fvSolution;
7 }
8 // * * * * *
9
10 // * * * * *
```

*system/fcSchemes:*

```

1 FoamFile
2 {
3     version      2.0;
4     format       ascii;
5     class        dictionary;
6     object       fvSchemes;
7 }
8 // * * * * *
9
10 ddtSchemes
11 {
12 }
13
14 gradSchemes
15 {
16 }
17
18 divSchemes
19 {
20 }
21
22 laplacianSchemes
23 {
24 }
25
26 interpolationSchemes
27 {
28 }
29
30 snGradSchemes
31 {
32 }
33
34 fluxRequired
35 {
36 }
37
38
39 // * * * * *
```

And last the *controlDict* is:

```

1 application      chtMultiRegionSimpleFoam;
2
3 startFrom        startTime;
4
5 startTime        0;
6
7 stopAt           endTime;
8
9 endTime          500;
10
11 deltaT           1;
```

```

12
13 writeControl    timeStep;
14
15 writeInterval   100;
16
17 purgeWrite      10;
18
19 writeFormat      ascii;
20
21 writePrecision   7;
22
23 writeCompression uncompressed;
24
25 timeFormat       general;
26
27 timePrecision    6;
28
29 runTimeModifiable true;
30
31
32 // ***** //

```

## 2.3 Running the simulation

First let's summarize all the commands used for the preprocessing:

```

blockMesh
topoSet
splitMeshRegions -cellZones -overwrite

changeDictionary -region leftSolid
changeDictionary -region rightSolid
changeDictionary -region topSolid

```

After the preprocessing is complete the simulation can begin with:

```
foamJob -screen chtMultiRegionSimpleFoam
```

## 2.4 Post-processing

Once the results are ready the user can launch *paraview* to visualize the results in the same manner as the explained in 2.2.3 to visualize the mesh, remembering the *.OpenFOAM* file of each region can be generated with the *paraFoam -touchAll* command, but it's not necessary to repeat this step if the files are already present.

Once loaded in *paraview* each region is handled separately but they can be grouped by selecting all of them (clicking on them while holding the *Ctrl* key) and using the *Group Datasets* filter. Several *GroupDatasets* entities appear within the *Pipeline Browser* which can be selected to handle all the regions as one (Figure 15), this is necessary to plot a field over a line crossing multiple regions.

Before grouping it's important to note the *Volume Fields* and *Mesh Parts* the user wants to load need to be selected individually first, from the *Properties* menu of each region, and

then click *Apply*.

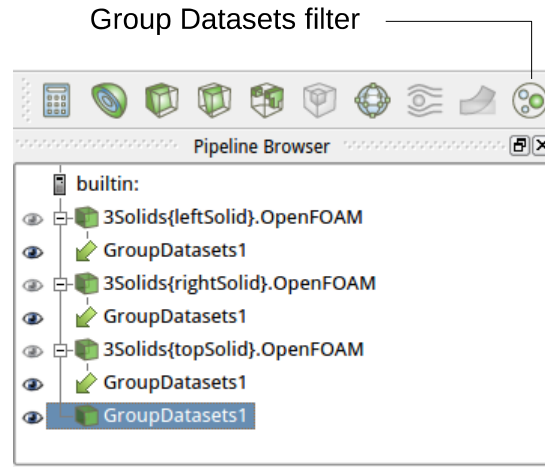


Figure 15: Group Datasets filter.

Besides *paraview* there's another very useful post-processing tool for heat transfer problems, that calculates the global heat rates (W) and the local heat fluxes (W/m<sup>2</sup>) through the wall faces of a region, this can help confirming the convergence and validating the results. It is executed by typing in the terminal:

```
wallHeatFlux -latestTime -region nameOfRegion
```

With this the terminal will output the boundary heat rates of the region “*nameOfRegion*” for the solution stored in the last time-folder (if the *latestTime* argument is used). Also inside the pertinent region-folder of this last time-folder a *wallHeatFlux* file is created containing the normal heat flux at each boundary patch cell, which can be post-processed with *paraview* as well.

The obtained heat rates are exposed in the next table:

Face position [m]	Heat rate [W]		
	leftSolid	rightSolid	topSolid
X = 0	-152.5	/	-87.37
X = 0.6	135.6	-135.7	/
X = 0.9	/	105.0	-0.1108
Y = 0	0.000	0.000	/
Y = 0.25	16.84	30.64	-47.52
Y = 0.5	/	/	135.0
Σ	-0.1	-0.1	0.0

Table 3: Heat rates through the boundary faces of each region. Positive values for a heat flux entering the region.



Overall the error is low which is a sign of good convergence and the results look consistent with the physics of the case.

*Note: Notice even though this is a 2D case the mesh is a 3D block and the total heat rates are computed by integrating the heat fluxes over the finite area of the mesh (for this reason the z-dimension of the mesh was conveniently set to 1m). The average heat flux can be obtained by simply dividing the heat rate by this area.*

To conclude the chapter here are some other results from paraview.

Temperature distribution on the leftSolid ( $\kappa = 210\text{W}/(\text{m}\cdot\text{K})$ ):

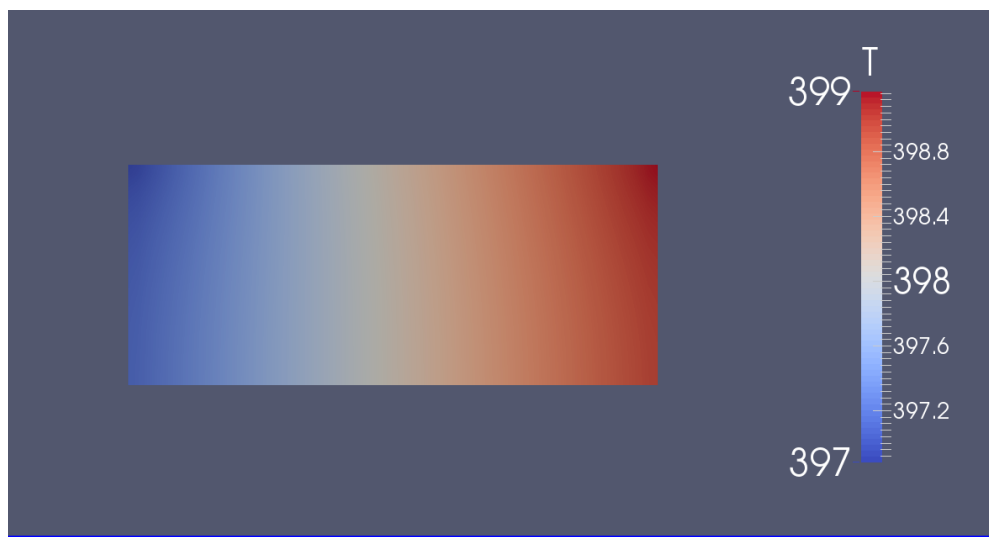


Figure 16: Temperature distribution on the leftSolid region (material 2)

In Figure 17 the temperature distribution on the whole domain. The temperature of the leftSolid may look constant but as Figure 16 showed that's because it has a much smaller temperature gradient (because of the higher thermal conductivity) and so the small temperature differences not appreciated due to the wider data range of this representation.

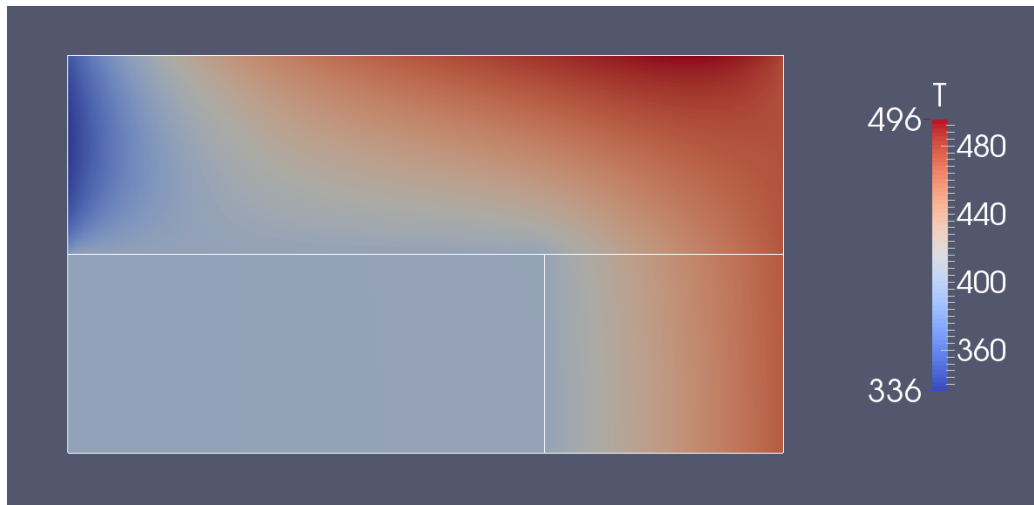


Figure 17: Temperature distribution on the whole domain

Temperature vs. x-coordinate at the  $y=0.2\text{m}$  plane. Hence from  $x=0$  to  $0.6\text{m}$  it corresponds to the *leftSolid* and from  $0.6$  to  $0.9\text{m}$  the *rightSolid*. It highlights the difference in temperature gradients.

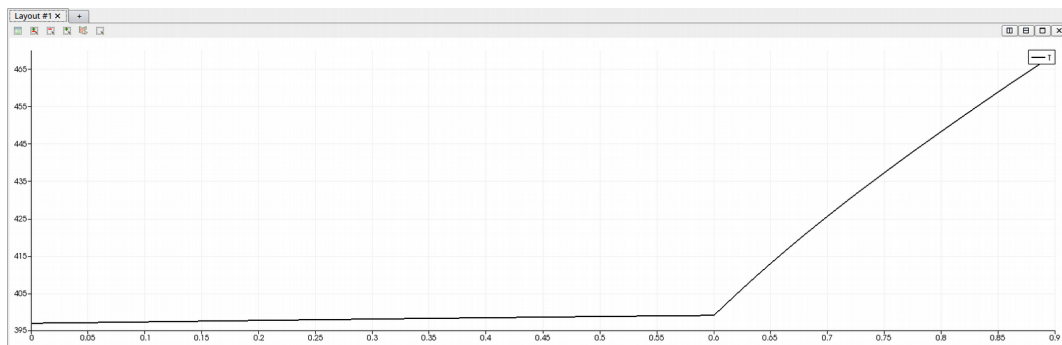


Figure 18: Temperature [K] vs.  $x$  [m] across the  $y=0.2\text{m}$  plane.

# Chapter 3 - Convection

This chapter explains the implementation of thermal convection for its resolution with `buoyantSimpleFoam` and `buoyantPimpleFoam`, the steady-state and transient solvers for compressible, convective flows. These solvers are chosen because they are the most general and because they resolve the flow in the same way as the *cht solvers*, hence together with Chapter 2 this chapter also establishes the base for the resolution of conjugate heat transfer problems.

However the problems presented in this chapter could also be resolved with slight modifications under the incompressible flow assumption with the Boussinesq approximation using the `buoyantBoussinesqSimpleFoam` and `buoyantBoussinesqPimpleFoam` solvers.

The Part B of this chapter also introduces *snappyHexMesh*, a powerful meshing utility very useful for meshing complex geometries.

## 3.1 Part A: Forced convection

### 3.1.1 Description of the case

This first part of the chapter will study the convective heat transfer for a case of external, forced convection of dry air over an isothermal, horizontal, semi-infinite plate. Therefore unlike the previous chapters now only the fluid domain will be resolved, with a boundary conditioned by the plate.

Figure 19 shows the configuration of the problem. The plate has a length of 0.5m and it's kept at constant 600K. The upstream flow has a velocity of 5m/s, a temperature of 300K and a pressure of 101325Pa (1 atm). The thermo-physical properties of the fluid are assumed constant and evaluated at the film temperature (450K), they are indicated in Table 4.

$c_p$ [J/(kg·K)]	$\mu$ [ $10^{-5}$ kg/(m·s)]	$\kappa$ [W/(m·K)]	$Pr$
1028	2.484	0.03713	0.6878

Table 4: Thermo-physical properties of the fluid (dry air).

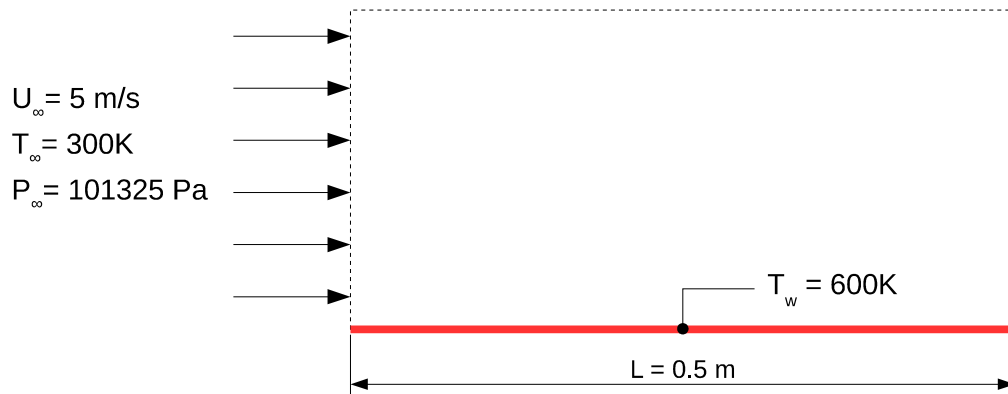


Figure 19: Schematic of the problem.

### 3.1.1.1 Assumptions

- Steady-state conditions.
- Bi-dimensional, compressible, laminar flow
- Newtonian fluid
- Perfect gas
- Constant thermo-physical properties
- Negligible radiation effects

### 3.1.1.2 Formulation

The fundamental governing equations of the problem are the three conservation laws of mass, momentum and energy.

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

Conservation of momentum:

$$\rho \frac{D\vec{u}}{Dt} = -\nabla \cdot p + \nabla \cdot \vec{\tau} + \rho \cdot \vec{g}$$

Where  $\tau$  is the deviatoric stress tensor, for a compressible, Newtonian fluid this is:

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}$$

And conservation of energy:

$$\rho \frac{Dh}{Dt} + \rho \frac{De_c}{Dt} = \frac{\partial p}{\partial t} + \nabla \cdot (\kappa \nabla T) + \rho q_v + \nabla \cdot (\vec{\tau} \cdot \vec{u}) + \rho \vec{g} \cdot \vec{u}$$

Where  $e_c$  is the specific kinematic energy:

$$e_c = \frac{1}{2} |\vec{u}|^2$$

Since there aren't neither internal heat sources nor radiation interacting with the medium the volumetric heat flux term,  $q_v$ , is zero, and because it's a steady-state problem there's no time dependence so the temporal derivatives are null as well. Hence the previous equations can be simplified to:

$$\nabla \cdot (\rho \vec{u}) = 0$$

$$\rho (\vec{u} \cdot \nabla \vec{u}) = - \nabla \cdot p + \nabla \cdot \vec{\tau} + \rho \cdot \vec{g}$$

$$\rho (\vec{u} \cdot \nabla h + \vec{u} \cdot \nabla e_c) = \frac{\partial p}{\partial t} + \nabla \cdot (\kappa \nabla T) + \nabla \cdot (\vec{\tau} \cdot \vec{u}) + \rho \vec{g} \cdot \vec{u}$$

And the perfect gas assumption provides this two additional relations:

$$pV = nRT \quad h = c_p T$$

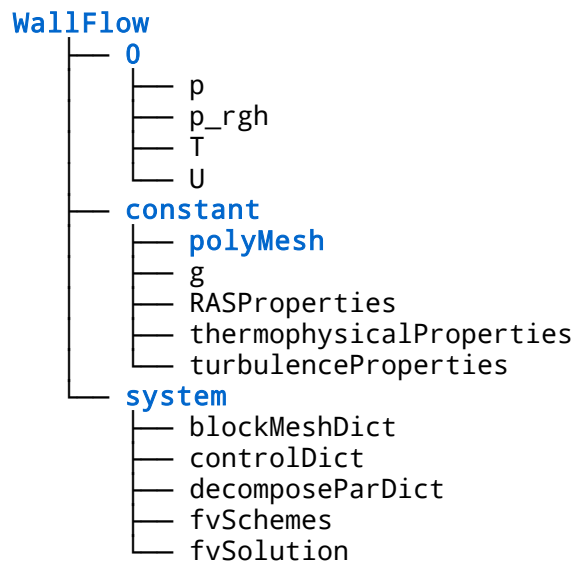
Finally, the laminar to turbulent transition is characterized by the Reynolds number and it happens around  $Re_x = 5 \cdot 10^5$ , where the characteristic length is the traveled distance over the plate. For the proposed case the maximum Reynolds is:

$$Re_L = \frac{\rho U_\infty L}{\mu} = \frac{0.7846 \cdot 5 \cdot 0.5}{2.484 \cdot 10^{-5}} = 78974$$

Which is still below the critical Reynolds so the assumption of laminar flow is consistent.

### 3.1.2 Preprocessing

Structure of the case:



#### 3.1.2.1 Mesh Generation

The mesh is generated using *blockMesh* with the following *blockMeshDict*:

```

1  convertToMeters 1;
2
3  vertices
4  (
5      (0 0 0)
6      (0.5 0 0)
7      (0.5 0.2 0)
8      (0 0.2 0)
9      (0 0 1)
10     (0.5 0 1)
11     (0.5 0.2 1)
12     (0 0.2 1)
13 );
14
15 blocks
16 (
17     hex (0 1 2 3 4 5 6 7) (100 100 1)
18     simpleGrading (1 40 1)
19 );
20
21 edges
22 (
23 );
24
25 boundary
26 (
27     maxY
28     {
29         type symmetryPlane;
30         faces
31         (
32             (3 7 6 2)
33         );
34     }
35     inlet
36     {
37         type patch;
38         faces
  
```

```

39      (
40      (0 4 7 3)
41      );
42    }
43    outlet
44    {
45      type patch;
46      faces
47      (
48      (2 6 5 1)
49      );
50    }
51    minY
52    {
53      type wall;
54      faces
55      (
56      (1 5 4 0)
57      );
58    }
59  );
60
61  mergePatchPairs
62  (
63  );
64
65  // ***** //

```

The height of the domain is chosen so the upper patch is far enough from the developing flow that a zeroGradient condition for the velocity can be considered physically accurate and can be applied on that patch later.

Also this case takes advantage of the grading functionality, applying a grading of 40 on the y-direction (thus  $40 = [\text{top cells height}] / [\text{bottom cells height}]$ ) to concentrate more cells near the wall. Figure 20 and Figure 21 show the resulting mesh.

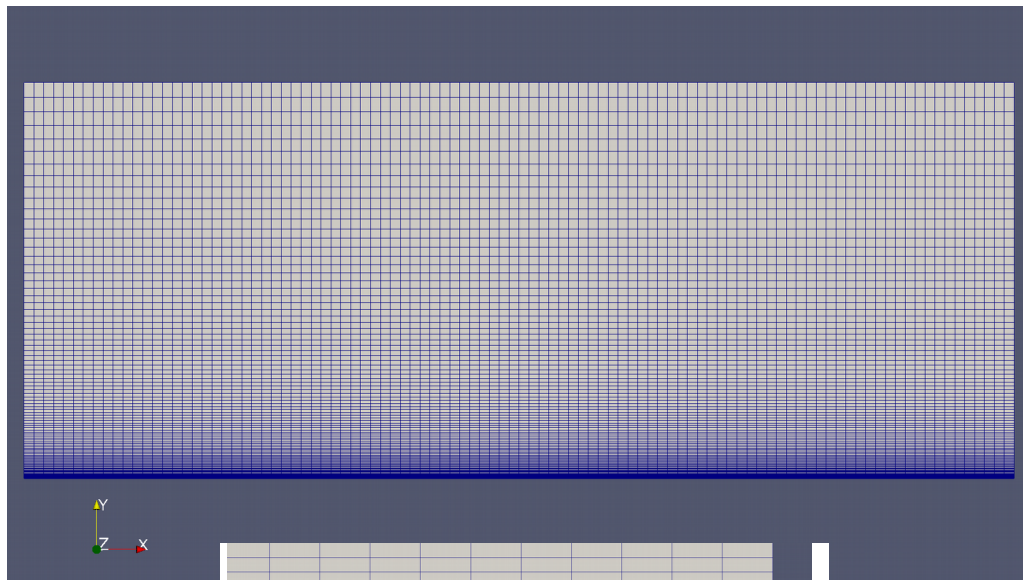


Figure 20: Visualiza

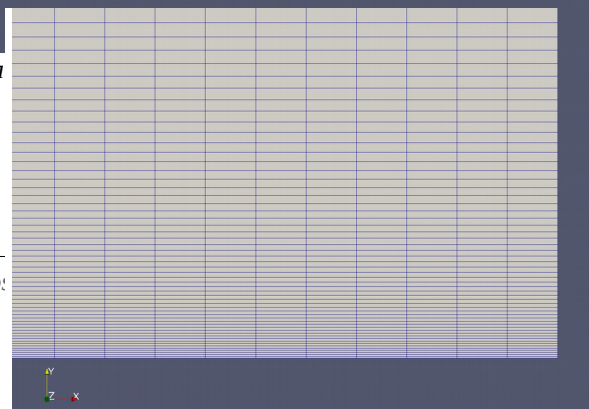


Figure 21: Detail of the graded region.

### 3.1.2.2 Boundary conditions

This case uses four files for the initial boundary conditions:  $T$  (temperature),  $U$  (velocity) and  $p$  (pressure) and  $p\_rgh$  (pressure -  $\rho gH$ ) which is simply the pressure without the hydrostatic contribution and simplifies the definition of the pressure boundaries.

$T$ :

```

1  imensions      [0 0 0 1 0 0 0];
2
3  internalField  uniform 300;
4
5  boundaryField
6  {
7      maxY
8      {
9          type      inletOutlet;
10         inletValue  uniform 300;
11         value       uniform 300;
12     }
13     inlet
14     {
15         type      fixedValue;
16         value      uniform 300;
17     }
18     outlet
19     {
20         type      zeroGradient;
21     }
22     minY
23     {
24         type      fixedValue;
25         value      uniform 600;
26     }
27
28     defaultFaces
29     {
30         type      empty;
31     }
32 }
33
34 // ***** //
```

$U$ :

```

1  dimensions      [0 1 -1 0 0 0 0];
2
3  internalField  uniform (5 0 0);
4
5  boundaryField
6  {
7      maxY
8      {
9          type      zeroGradient;
10     }
11     minY
12     {
13         type      fixedValue;
14         value      uniform (0 0 0);
15     }
16     inlet
17     {
18         type      fixedValue;
19         value      uniform (5 0 0);
20     }
21     outlet
22     {
23         type      inletOutlet;

```



```

24     inletValue      uniform (0 0 0);
25     value           uniform (5 0 0);
26 }
27
28     defaultFaces
29     {
30         type         empty;
31     }
32 }
33
34 // *****

```

The boundary conditions of temperature and velocity on the `inlet`, and `minY` patches are self-explanatory. Since  $U$  is a vector the corresponding values are defined by the three components of the vector.

On the outlet the `inletOutlet` type is used for the velocity, this type works as a `fixedValue` if the flow enters the domain (using the `inletValue`) and as a `zeroGradient` if it exits it, in this case it is used to avoid reverse flow as it's not expected, this can improve the stability of the resolution. On the `maxY` patch the velocity uses `zeroGradient` as explained previously and the `inletOutlet` type is used for the temperature, this is recommended for patches where it's unclear whether the flow will enter or exit the domain or where both things can happen.

*p\_rgh:*

```

1  dimensions      [1 -1 -2 0 0 0 0];
2
3  internalField    uniform 101325;
4
5  boundaryField
6  {
7      maxY
8      {
9          type      fixedValue;
10         value      $internalField;
11     }
12     minY
13     {
14         type      fixedFluxPressure;
15         value      $internalField;
16     }
17     inlet
18     {
19         type      fixedFluxPressure;
20         value      $internalField;
21     }
22     outlet
23     {
24         type      fixedValue;
25         value      $internalField;
26     }
27
28     defaultFaces
29     {
30         type      empty;
31     }
32 }
33
34 // *****

```

*p:*

```

1  dimensions      [1 -1 -2 0 0 0 0];
2
3  internalField    uniform 101325;
4
5  boundaryField
6  {
7      ".*"
8      {
9          type      calculated;
10         value      $internalField;
11     }
12
13     defaultFaces
14     {
15         type      empty;
16     }
17 }
18
19 // *****

```

As for the pressure, since the pressure boundaries are defined through  $p\_rgh$ ,  $p$  is left as *calculated* at all patches aside from those entirely defined by the geometric condition (such as *empty* or *symmetryPlane*). With this,  $p$  is simply computed as  $p = p\_rgh + \rho gH$

The field  $p\_rgh$  uses a *fixedFluxPressure* type for the *inlet* and *minY*, this adjusts the gradient according to the velocity at the boundary and is the usual type on patches where the velocity is known. At the *outlet* and *maxY* the pressure is specified through a *fixedValue* (101325).

These two files make use of the keyword *\$internalField* for the *value* entries, this instructs OpenFOAM to use the same value as the one specified in *internalField* which can be a more convenient.

### 3.1.2.3 Properties

The thermo-physical properties are defined with the *thermophysicalProperties* dictionary in a similar way as the previous chapter but using a model for a perfect gas with constant properties:

```

1  thermoType
2  {
3      type      heRhoThermo;
4      mixture    pureMixture;
5      transport  const; //constant mu and Pr
6      thermo     hConst; //constant Cp
7      equationOfState perfectGas;
8      specie     specie;
9      energy     sensibleEnthalpy;
10 }
11
12
13 mixture
14 {
15     specie
16     {
17         nMoles      1;
18         molWeight    28.9;
19     }
20     thermodynamics

```

```

21     {
22         Cp          1028.3;
23         Hf          0;
24     }
25     transport
26     {
27         mu          2.484e-05;
28         Pr          0.6878;
29     }
30 }

```

In addition there are two new dictionaries used for the determination of the turbulence model which have to be set to laminar.

*turbulenceProperties:*

```

1  simulationType  laminar;
2
3
4  // ***** //

```

*RASProperties:*

```

1  RASModel      laminar;
2
3  turbulence     off;
4
5  printCoeffs   on;
6
7
8  // ***** //

```

Finally, the file named *g* determines the direction and magnitude of the gravitational acceleration:

```

1  dimensions     [0 1 -2 0 0 0 0];
2  value          ( 0 -9.81 0 );
3
4  // ***** //

```

### 3.1.2.4 Control, Solution and Schemes

*fvSolution:*

```

1  solvers
2  {
3      p_rgh
4      {
5          solver          GAMG;
6          tolerance       1e-7;
7          relTol          0.01;
8
9          smoother        DICGaussSeidel;
10
11         cacheAgglomeration true;
12         nCellsInCoarsestLevel 100;
13         agglomerator      faceAreaPair;
14         mergeLevels       1;
15         maxIter           100;
16     }
17
18     "(u|h)"

```

```

19     {
20         solver          PBiCG;
21         preconditioner  DILU;
22         tolerance       1e-7;
23         relTol          0.01;
24     }
25 }
26
27 SIMPLE
28 {
29     momentumPredictor no;
30     nNonOrthogonalCorrectors 0;
31     pRefCell          0;
32     pRefValue          0;
33
34 }
35
36
37 relaxationFactors
38 {
39     rho          1;
40     p_rgh        0.7;
41     U            0.7;
42     h            0.7;
43 }

```

*fvSchemes:*

```

1  ddtSchemes
2  {
3      default          steadyState;
4  }
5
6  gradSchemes
7  {
8      default          Gauss linear;
9  }
10
11 divSchemes
12 {
13     default            bounded Gauss upwind;
14     div((muEff*dev2(T(grad(U)))) Gauss linear;
15 }
16
17 laplacianSchemes
18 {
19     default            Gauss linear uncorrected;
20 }
21
22 interpolationSchemes
23 {
24     default            linear;
25 }
26
27 snGradSchemes
28 {
29     default            uncorrected;
30 }
31
32 fluxRequired
33 {
34     default            no;
35     p_rgh;
36 }
37
38
39 // *****

```

A very general guideline for the *fvSchemes* dictionary, when dealing with compressible

flows, is to begin the simulations with a first order (upwind) default scheme under `divSchemes`, bounded for steady-state simulations and unbounded for transient, as higher order schemes can cause stability issues.

*controlDict*:

```

1  application      buoyantSimpleFoam;
2
3  startFrom        latestTime;
4
5  startTime        0;
6
7  stopAt           endTime;
8
9  endTime          1500;
10
11 deltaT           1;
12
13 writeControl      runtime;
14
15 writeInterval     250;
16
17 purgeWrite        0;
18
19 writeFormat        ascii;
20
21 writePrecision     9;
22
23 writeCompression  off;
24
25 timeFormat         general;
26
27 timePrecision      6;
28
29 runtimeModifiable true;
30
31 adjustTimeStep     no;
32
33 maxCo              1;
34
35 // ***** //
```

### 3.1.3 Running the simulation in parallel

OpenFOAM supports parallel processing by using the method known as domain decomposition, this can significantly reduce the computation time when multiple processors are available. With this method the domain is divided into several sub-domains which can be allocated to different processors for solution. The process involves the decomposition of the case, the resolution of the decomposed case and the posterior recomposition in order to normally post-process the results.

To decompose it the *decomposeParDict* dictionary is needed to specify how the domain is divided:

```

1  numberOfSubdomains 4;
2  method simple;
3  simpleCoeffs
4  {
5      n ( 2 2 1); //x y z
6      delta 0.001;
7  }
8
```

```

9      distributed false;
10     roots
11     (
12     );
13
14 // *****

```

In `numberOfSubdomains` the total number of sub-domains is specified. With the `simple` method the domain is divided by direction into pieces with a similar number of cells, the number of divisions in each direction is given at the entry in line 5. `delta` is a parameter known as cell skew factor, typically set to  $10^{-3}$ .

Next, to decompose the case the user has to run from the terminal:

```
decomposePar
```

After that several “processor-files” (`processor0`, `processor1`...) will appear within the case directory, one for each sub-domain. This step has to be repeated every time the mesh or the boundary conditions are modified. For this reason using the `force` argument can be useful as this will automatically replace any preexisting processor file:

```
decomposePar -force
```

Now the case is ready to run in parallel, in order to begin the parallel execution in a local machine the following command can be used:

```
foamJob -screen -parallel <name of the solver>
```

In this case:

```
foamJob -screen -parallel buoyantSimpleFoam
```

Lastly, after the computation has finished, the case can be reconstructed with the command below, leaving it ready for a normal post-processing:

```
reconstructPar
```

### 3.1.4 Post-processing

This case can be validated by comparing the Nusselt number with the ones obtained through empirical correlations found in the literature. For an isothermal horizontal plate under a forced, laminar flow the following one is proposed in *Fundamentals of Heat and Mass Transfer (Incropera et al. 2011 [1])*:

$$\overline{Nu}_x = 0.664 \cdot Re_x^{(1/2)} \cdot Pr^{(1/3)}$$

As for the Nusselt of the simulated case it can be obtained using `wallHeatFlux` since:

$$\dot{q} = \bar{h} A (T_w - T_f) = \frac{\overline{Nu}_L \cdot \kappa}{L} A (T_w - T_f)$$

Where  $L$  is the total length of the plate and  $T_w - T_f$  the difference between the temperature of the plate ( $T_w$ ) and the temperature of the flow far from the plate ( $T_f$ ).

The results are summarized in Table 5. The obtained Nusselt is a 10.53% greater than the one of the correlation which, considering empirical correlations may not be very accurate, is a good enough result to validate the case.

Simulation heat rate [W]	Simulation $\overline{Nu}_L$	Correlation $\overline{Nu}_L$	Simulation/Correlation [%]
2028.0	182.06	164.72	10.53

Table 5: Comparison between the average Nusselt numbers obtained from the simulation and the empirical correlation.

To end, next are some more results post-processed with paraFoam using the basic tools explained in the previous chapters.

Magnitude of the velocity of the flow. Close to the wall the laminar boundary layer starts developing:

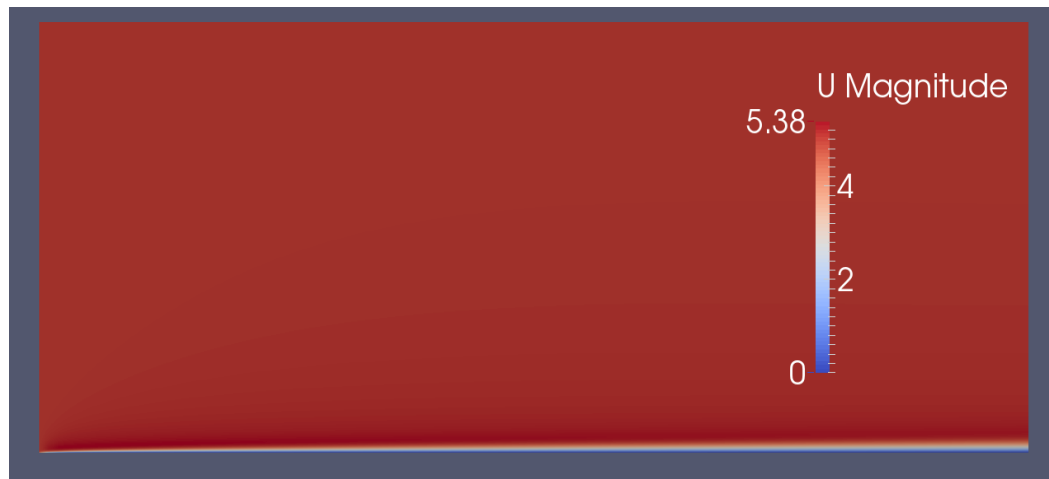


Figure 22: Magnitude of the velocity of the flow over the whole domain.

Temperature distribution near the wall at the right end. The thermal boundary layer can be appreciated as well:

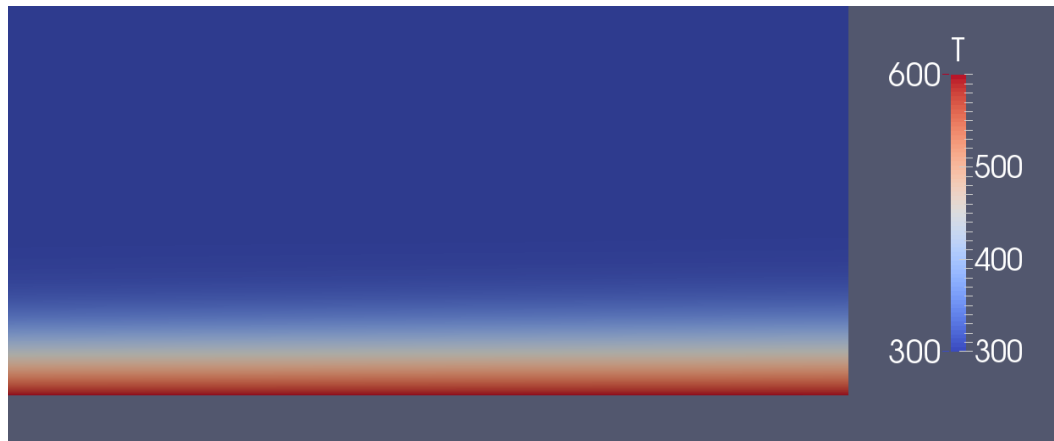


Figure 23: Detail of the temperature distribution close to the wall at the right end.

Temperature and velocity profiles near the wall at  $x=0.25\text{m}$ :

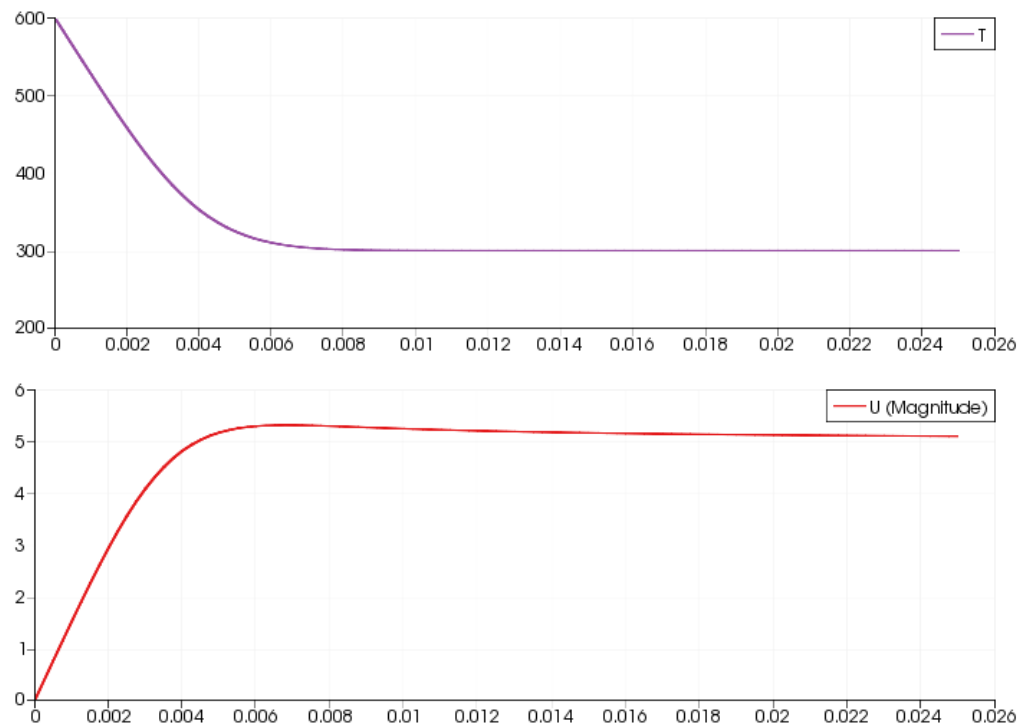


Figure 24: Temperature [K] vs.  $y$  [m] (up) and velocity [m/s] vs.  $y$  [m] (down) at  $x=0.25\text{m}$ .



## 3.2 Part B: Natural convection

### 3.2.1 Description of the case

In this second part of the chapter a transient, bi-dimensional case of natural convection of the air surrounding an isothermal, horizontal cylinder is presented.

The case consists on an horizontal cylinder with a wall temperature kept at a constant 500K, surrounded by an open volume of dry air at 1atm, initially quiescent and with a uniform temperature of 300K. The schematic below summarizes it.

The thermo-physical properties, assumed constant, are evaluated at the film temperature (400K). See Table 6.

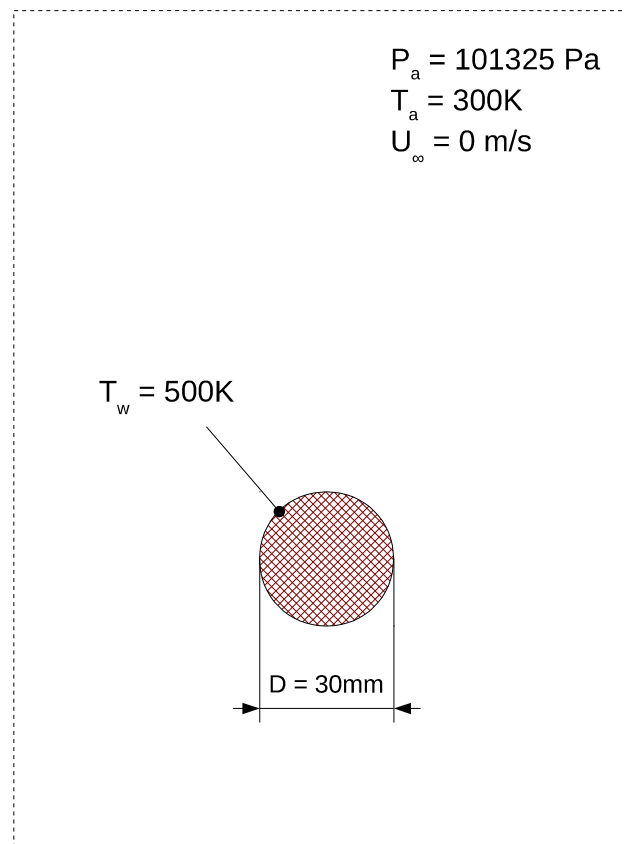


Figure 25: Schematic of the case.

$c_p \text{ [J/(kg}\cdot\text{K)]}$	$\mu \text{ [10}^{-5} \text{ kg/(m}\cdot\text{s)]}$	$\kappa \text{ [W/(m}\cdot\text{K)]}$	$Pr$
1021	2.285	0.03368	0.6929

Table 6: Thermo-physical properties of the fluid.

#### 3.2.1.1 Assumptions

- Bi-dimensional, compressible, laminar flow

- Newtonian fluid
- Perfect gas
- Constant thermo-physical properties
- Negligible radiation effects

### 3.2.1.2 Formulation

The governing equations are the same as in the previous part but since it's a transient case now the time dependent terms can't be eliminated.

Conservation of mass, momentum and energy:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\rho \frac{D\vec{u}}{Dt} = -\nabla \cdot p + \nabla \cdot \vec{\tau} + \rho \cdot \vec{g}$$

$$\rho \frac{Dh}{Dt} + \rho \frac{De_c}{Dt} = \frac{\partial p}{\partial t} + \nabla \cdot (\kappa \nabla T) + \nabla \cdot (\vec{\tau} \cdot \vec{u}) + \rho \vec{g} \cdot \vec{u}$$

And the ideal gas law with constant heat capacity, from the perfect gas assumption:

$$pV = nRT \quad h = c_p T$$

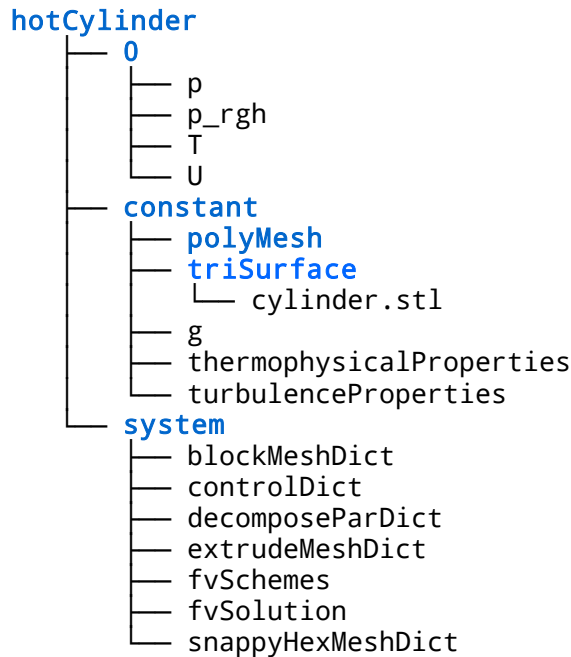
In addition, the steady-state solution of natural convection problems is characterized by the Rayleigh number, in this case:

$$Ra_D = \frac{g \beta (T_w - T_\infty) D^3}{\nu \alpha} = \frac{9.81 \cdot 2.5 \cdot 10^{-3} \cdot 200 \cdot 0.03^3}{2.589 \cdot 10^{-5} \cdot 3.737 \cdot 10^{-5}} = 1.369 \cdot 10^5$$

According to Kuehn T and Goldstein R (as cited by S.K.S. Boetcher, 2014 [3]) for Rayleigh numbers between  $10^4$  and  $10^8$  the flow forms a laminar boundary layer around the cylinder, so the calculated Rayleigh confirms the laminar flow assumption is in agreement. At higher Rayleigh numbers the flow becomes turbulent and at lower ones the heat transfer is dominated by conduction.

### 3.2.2 Preprocessing

Structure of the case:



#### 3.2.2.1 Mesh generation

This part will introduce *snappyHexMesh*, a powerful 3D meshing tool which can generate meshes based on STL or OBJ geometry files. The input geometry has to be located in *constant/triSurface*, in this case the *cylinder.stl* file, a 3D model of the central cylinder.

Since *snappyHexMesh* works in the 3 dimensions it will generate unnecessary divisions in the z-direction, this would slow the solution so another tool is used to correct that: *extrudeMesh*. This tool can create a mesh by extruding a face of the prior mesh generated with *snappyHexMesh*, hence by extruding one of the faces perpendicular to Z in the z-direction an equivalent mesh without z-divisions can be obtained.

Before using *snappyHexMesh* it's first necessary to generate a background mesh covering all the domain inside the air container. This is done as usual with *blockMesh*. The *blockMeshDict* is:

```

1  convertToMeters 0.001;
2
3  vertices
4  (
5      (-150 -150 0)
6      (150 -150 0)
7      (150 450 0)
8      (-150 450 0)
9      (-150 -150 10)
10     (150 -150 10)
11     (150 450 10)
12     (-150 450 10)
  
```

```

13 );
14
15 blocks
16 (
17     hex (0 1 2 3 4 5 6 7) (75 150 1) simpleGrading (1 1 1)
18 );
19
20 edges
21 (
22 );
23
24 boundary
25 (
26     Top
27     {
28         type patch;
29         faces
30         (
31             (3 7 6 2)
32         );
33     }
34     Bottom
35     {
36         type patch;
37         faces
38         (
39             (1 5 4 0)
40         );
41     }
42     sides
43     {
44         type patch;
45         faces
46         (
47             (2 6 5 1)
48             (0 4 7 3)
49         );
50     }
51     symFront
52     {
53         type empty;
54         faces
55         (
56             (4 5 6 7)
57         );
58     }
59     symBack
60     {
61         type empty;
62         faces
63         (
64             (0 3 2 1)
65         );
66     }
67 );
68
69 mergePatchPairs
70 (
71 );
72
73 // *****

```

This time the front and back empty faces are in separated patches so one of them can later be used for the extrusion.

Next let's see the instructions for *snappyHexMesh* in *snappyHexMeshDict*. Mastering *snappyHexMesh* requires time and experience, it is a very complex dictionary with lots of entries and only some of the basic features are going to be discussed in this guide,

```

1  castellatedMesh true;
2  snap           true;
3  addLayers      false;
4

```

This first part controls the three steps involved in the generation of the mesh. The first step refines the background hexahedra mesh according to some specifications and discards the part which doesn't belong to the domain (the internal part of the cylinder in this case). The second step morphs the mesh so the cells in contact with the geometry match its surface. The last can be used to add layer of cells over a surface. Figure 26 illustrates this:

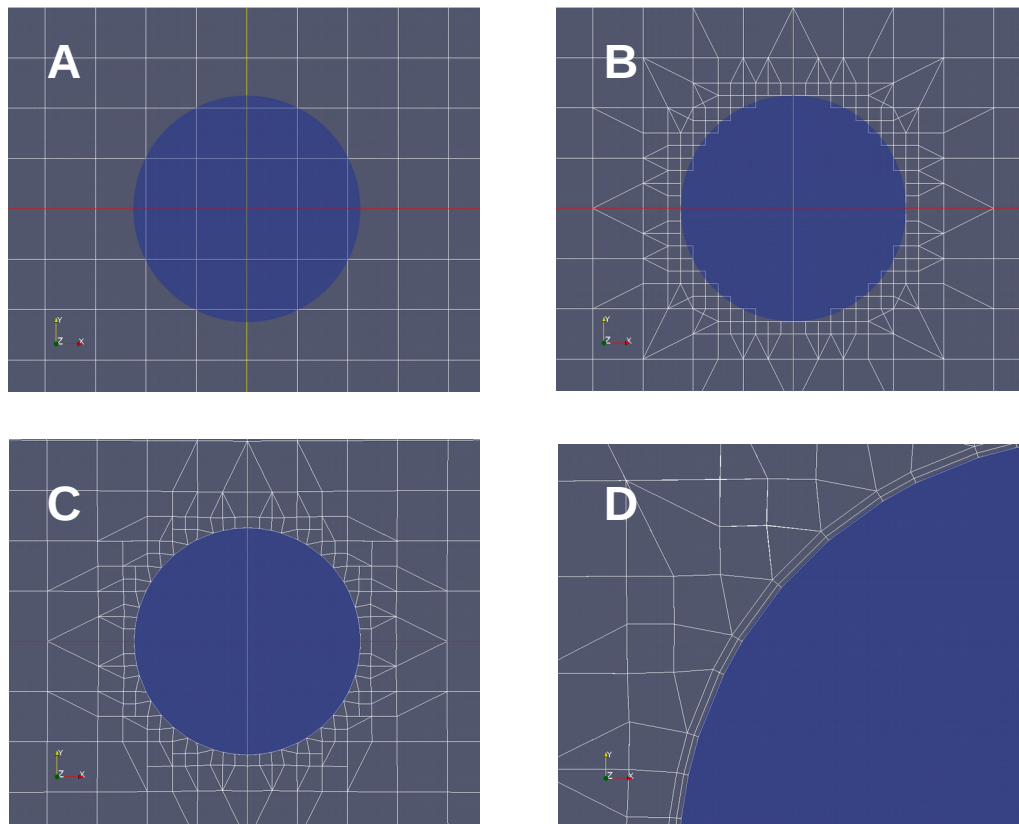


Figure 26: Example of meshing steps. A - Background mesh. B - Castellated mesh. C - Snapped mesh. D - Added layers.

The code follows with:

```

5  geometry
6  {
7    cylinder.stl
8    {
9      type triSurfaceMesh;
10     scale 0.001;
11     name cylinder;
12   }
13   refinementBox
14   {
15     type searchableBox;
16     min (-0.05 -0.1 -1);

```

```

17         max ( 0.05 1 1);
18     }
19
20 };
21

```

This part is used to indicate the STL file or files used for the refinement and the snapping. Since the file is in meter units the scale is set to 0.001 to convert to millimeter units. `name` defines the name of the corresponding boundary patch in the mesh.

In addition this section can be used to specify user-defined refinement regions, in this example this feature is used to define a box around the cylinder and the area where the plume is expected to further refine this region.

Next:

```

22 castellatedMeshControls
23 {
24     maxLocalCells 1000000;
25
26     maxGlobalCells 2000000;
27
28     minRefinementCells 10;
29
30     maxLoadUnbalance 0.10;
31
32     nCellsBetweenLevels 15;
33
34     features
35     (
36     );
37
38     refinementSurfaces
39     {
40         cylinder
41         {
42             level (4 4);
43
44             patchInfo
45             {
46                 type wall;
47             }
48         }
49     }
50
51     resolveFeatureAngle 30;
52
53     refinementRegions
54     {
55         refinementBox
56         {
57             mode inside;
58             levels ((0.05 1));
59         }
60     }
61
62     locationInMesh (0.052631 0.058706 0.001);
63
64     allowFreeStandingZoneFaces false;
65 }

```

These are the instructions related to the `castellatedMesh` step. Lines 38 to 49 define the surface based refinement, i.e. refinement based on the proximity to the geometry surface.

The refinement level is based on the background mesh, level 1 divides a background hexahedron by two in every dimension (resulting in 8 smaller parts) and each subsequent level does the same relative to the hexahedra of the previous level (Figure 27).

The minimum and maximum levels are specified next to the `level` keyword, the maximum level (at right) can be used to further refine where the local curvature angle is greater than `resolveFeatureAngle` but it can have a negative impact on the quality of the mesh and for this particular case is pointless because of the constant curvature. Below that, at `patchInfo`, the geometric type corresponding to the cylinder patch is specified.

Next, from line 53 to 60, there's the part related to the region-wise refinement. At `mode` it can be instructed to refine `inside` or `outside` the defined region or to refine based on a `distance` from the bounding surface. The first entry in `levels` is used to specify the distance on for `distance` mode so it has no effect in this example, and the second entry specifies the refinement level.

Finally, `locationInMesh` defines where the domain of interest is, either inside or outside the input geometry (the cylinder), so the program knows whether to keep the mesh inside or outside, thus a point outside the cylinder is defined. Furthermore the point must be within the domain but outside any cell face (even after the refinement), for that reason it's a good idea to add some random decimals to make it more unlikely for the point to be on a face.

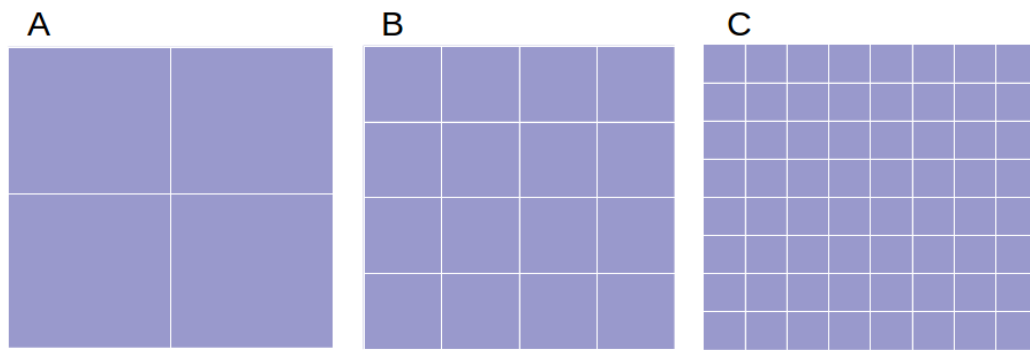


Figure 27: Refinement levels. A: Level 0 (background). B: Level 1. C: Level 2.

The remaining instructions control the `snap` step, the `addLayers` step and the quality of the mesh. They are as follows:

```

66 snapControls
67 {
68     nSmoothPatch 3;
69
70     tolerance 2.0;
71
72     nSolveIter 30;
73

```

```

74     nRelaxIter 5;
75
76         nFeatureSnapIter 10;
77
78         implicitFeatureSnap false;
79
80         explicitFeatureSnap true;
81
82         multiRegionFeatureSnap false;
83     }
84
85
86 addLayersControls
87 {
88     relativeSizes true;
89
90     layers
91     {
92
93     }
94
95     expansionRatio 2;
96
97     finalLayerThickness 0.5;
98
99     minThickness 0.001;
100
101     nGrow 0;
102
103     featureAngle 90;
104
105     slipFeatureAngle 30;
106
107     nRelaxIter 3;
108
109     nSmoothSurfaceNormals 1;
110
111     nSmoothNormals 3;
112
113     nSmoothThickness 10;
114
115     maxFaceThicknessRatio 0.5;
116
117     maxThicknessToMedialRatio 0.3;
118
119     minMedianAxisAngle 90;
120
121     nBufferCellsNoExtrude 0;
122
123     nLayerIter 50;
124 }
125
126 meshQualityControls
127 {
128     maxNonOrtho 65;
129
130     maxBoundarySkewness 20;
131
132     maxInternalSkewness 4;
133
134     maxConcave 80;
135
136     minVol 1e-13;
137
138     minTetQuality 1e-30;
139
140     minArea -1;
141
142     minTwist 0.05;
143
144     minDeterminant 0.001;
145
146     minFaceWeight 0.05;

```



```

147
148     minVolRatio 0.01;
149
150     minTriangleTwist -1;
151
152     nSmoothScale 4;
153
154     errorReduction 0.75;
155 }
156
157
158 // Advanced
159
160 mergeTolerance 1e-6;
161
162
163 // ***** //
```

The next step is to set up the *extrudeMeshDict*:

```

1  constructFrom patch;
2  sourceCase "$FOAM_CASE";
3  sourcePatches (symFront);
4
5  exposedPatchName symBack;
6
7  flipNormals false;
8
9  extrudeModel      linearNormal;
10
11  nLayers           1;
12
13  expansionRatio    1.0;
14
15  linearNormalCoeffs
16  {
17      thickness      1;
18  }
19
20  mergeFaces false;
21
22  mergeTol 0;
```

- **constructFrom patch:** Use a patch as a source for the extrusion
- **sourceCase:** The case where it will look for the specified patch. With “\$FOAM\_CASE” it uses the case where the dictionary is located.
- **sourcePatches:** The name of the patches to extrude.
- **exposedPatchName:** The name of the patch opposed to the extruded one.
- **extrudeModel linearNormal:** Extrude in the direction normal to the patch.
- **nLayers:** Number of divisions in the extruded direction.
- **thickness:** Length of the extrusion.

Once *blockMeshDict*, *snappyHexMeshDict* and *extrudeMeshDict* are set up the mesh is ready to be generated by executing:

```

blockMesh
snappyHexMesh -overwrite
extrudeMesh

```

As always, it is recommended to check the mesh with `checkMesh` and `paraFoam`.

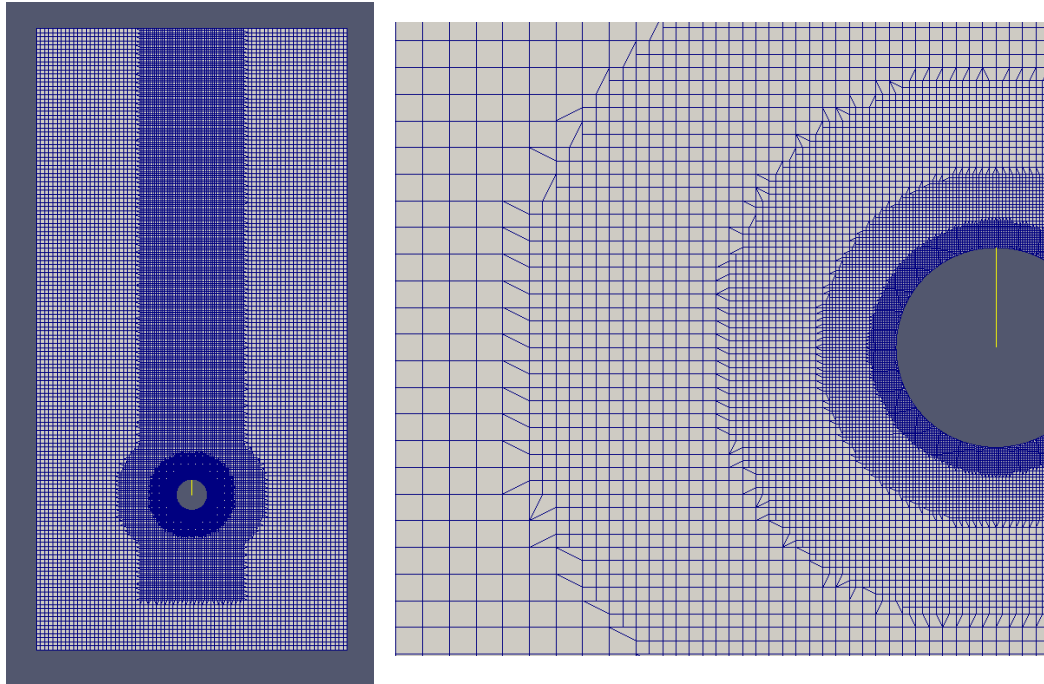


Figure 28: Overview of the mesh (left) and detail of the mesh near the cylinder (right).

### 3.2.2.2 Initial and boundary conditions

Setting the proper boundary conditions for open natural convection cases can be a delicate matter, a strategy used in this case is to place the boundary patches far from the cylinder in order to minimize their effect around the cylinder. The upper patch leaves an even more generous distance in order to let the thermal plume (i.e. the rising stream of hot air) develop properly.

On the `sides` and `Bottom` patches `totalPressure` and `pressureInletOutletVelocity` are used for `p_rgh` and `U` respectively. The first one establishes a constant total pressure ( $p_0$ ) condition and the second is a velocity condition meant for patches where the pressure is specified (if the flow enters the domain it derives the normal velocity from the mass flux and otherwise it acts as a `ZeroGradient`). The `Top` patch will be crossed by the plume so as to not disturb it `fixedFluxPressure` (`p_rgh`) and `zeroGradient` (`U`) are used instead.

As for the temperature, on all these external patches it takes advantage of the flexibility of the `inletOutlet` condition.

The boundary conditions on the cylinder wall are the usual ones.

*U:*

```

1  dimensions      [0 1 -1 0 0 0 0];
2
3  internalField    uniform (0 0 0);
4
5  boundaryField
6  {
7      sides
8      {
9          type      pressureInletOutletVelocity;
10         value      uniform (0 0 0);
11     }
12
13     Top
14     {
15         type      zeroGradient;
16     }
17     Bottom
18     {
19         type      pressureInletOutletVelocity;
20         value      uniform (0 0 0);
21     }
22     cylinder
23     {
24         type      fixedValue;
25         value      uniform (0 0 0);
26     }
27
28     symFront
29     {
30         type      empty;
31     }
32     symBack
33     {
34         type      empty;
35     }
36 }
37
38 // ***** //
```

*p\_rgh:*

```

1  dimensions      [1 -1 -2 0 0 0 0];
2
3  internalField    uniform 101325;
4
5  boundaryField
6  {
7      sides
8      {
9          type      totalPressure;
10         p0         $internalField;
11         U          U;
12         phi        phi;
13         rho        rho;
14         psi        none;
15         gamma      1.4;
16         value      $internalField;
17     }
18     Top
19     {
20         type      fixedFluxPressure;
21         value      $internalField;
22     }
23     Bottom
24     {
25         type      totalPressure;
26         p0         $internalField;
27         U          U;
28         phi        phi;

```

```

29         rho          rho;
30         psi          none;
31         gamma        1.4;
32         value        $internalField;
33     }
34
35     cylinder
36     {
37         type          fixedFluxPressure;
38         value        $internalField;
39     }
40
41     symFront
42     {
43         type          empty;
44     }
45     symBack
46     {
47         type          empty;
48     }
49 }
50
51 // *****

```

*T:*

```

1  dimensions      [0 0 0 1 0 0 0];
2
3  internalField   uniform 300;
4
5  boundaryField
6  {
7      "."
8      {
9          type          inletOutlet;
10         inletValue     uniform 300;
11     }
12     cylinder
13     {
14         type          fixedValue;
15         value         uniform 500;
16     }
17
18     symFront
19     {
20         type          empty;
21     }
22     symBack
23     {
24         type          empty;
25     }
26 }
27
28 // *****

```

*p:*

```

1  dimensions      [1 -1 -2 0 0 0 0];
2
3  internalField   uniform 101325;
4
5  boundaryField
6  {
7      "."
8      {
9          type          calculated;
10         value         $internalField;
11     }
12 }

```

```

13     symFront
14     {
15         type            empty;
16     }
17     symBack
18     {
19         type            empty;
20     }
21 }
22
23 // *****

```

### 3.2.2.3 Properties

With the previous part as a reference the *thermophysicalProperties* dictionary is simply updated with the new properties and the rest is kept the same.

*thermophysicalProperties*:

```

1  thermoType
2  {
3      type            heRhoThermo;
4      mixture         pureMixture;
5      transport       const;
6      thermo          hConst;
7      equationOfState perfectGas;
8      specie          specie;
9      energy          sensibleEnthalpy;
10 }
11
12
13 mixture
14 {
15     specie
16     {
17         nMoles        1;
18         molWeight     28.9;
19     }
20     thermodynamics
21     {
22         Cp            1021.1;
23         Hf            0;
24     }
25     transport
26     {
27         mu            2.285e-05;
28         Pr            0.6929;
29     }
30 }
31
32
33 // *****

```

### 3.2.2.4 Control, solution and schemes

When numerically solving transient flows an important stability criterion is the Courant–Friedrichs–Lewy (CFL) condition which establishes that for the solution to converge is necessary that:

$$C = \Delta t \sum_{i=1}^n \frac{u_{x_i}}{\Delta x_i} \leq C_{max}$$

Where:

- $C$  is known as the Courant number.
- $u_{x_i}$  is the component of the velocity in the  $x_i$  dimension.
- $\Delta t$  is the time interval.
- $\Delta x_i$  is the length interval.

The value of  $C_{\max}$  depends on the methods used for the solution, for explicit methods it's typically 1. OpenFOAM uses implicit/semi-implicit methods which allow greater  $C_{\max}$  values, nevertheless values of the order of 1 are advised to ensure the stability and precision when solving unsteady flows.

The CFL condition puts a limitation on the selected time-step but the maximum Courant number has to be estimated first. There's also the possibility to let the algorithm automatically adjust the time-step by specifying the desired  $C_{\max}$ , a very useful feature. This is done through the `controlDict` by setting `yes` on `adjustTimeStep` and introducing the  $C_{\max}$  on `maxCo` (see below, lines 31 and 33).

`controlDict`:

```

1  application      buoyantPimpleFoam;
2
3  startFrom        latestTime;
4
5  startTime        0;
6
7  stopAt           endTime;
8
9  endTime          5;
10
11 deltaT           1e-4;
12
13 writeControl      adjustableRunTime;
14
15 writeInterval     0.1;
16
17 purgeWrite       0;
18
19 writeFormat       ascii;
20
21 writePrecision    9;
22
23 writeCompression off;
24
25 timeFormat        general;
26
27 timePrecision     6;
28
29 runtimeModifiable true;
30
31 adjustTimeStep    yes;
32
33 maxCo             1;
34
35 // ***** //
```

Since the time-step is variable the `writeControl` is set to `adjustableRunTime` mode, it works in a similar way as `runTime` but it readjusts the time-step to make it exactly coincide with the `writeInterval` (0.2 seconds of simulated time), while `runTime` would write the result of the closest solved time.

The `fvSchemes` and `fvSolution` dictionaries also have some differences respect to the previous part:

*fvSchemes:*

```

1 ddtSchemes
2 {
3     default          Euler;
4 }
5
6 gradSchemes
7 {
8     default          Gauss linear;
9 }
10
11 divSchemes
12 {
13     default          none;
14     div(phi,U)       Gauss upwind;
15     div(phi,h)       Gauss upwind;
16     div(phi,K)       Gauss linear;
17     div((muEff*dev2(T(grad(U)))) Gauss linear;
18 }
19
20 laplacianSchemes
21 {
22     default          Gauss linear corrected;
23 }
24
25 interpolationSchemes
26 {
27     default          linear;
28 }
29
30 snGradSchemes
31 {
32     default          corrected;
33 }
34
35 fluxRequired
36 {
37     default          no;
38     p_rgh;
39 }
40
41
42 // ***** //
```

*fvSolution:*

```

1 solvers
2 {
3     "rho.*"
4     {
5         solver          PCG;
6         preconditioner  DIC;
7         tolerance       0;
8         relTol          0;
9     }
10
11     p_rgh
```

```

12     {
13         solver          PCG;
14         preconditioner   DIC;
15         tolerance        1e-8;
16         relTol           0.01;
17     }
18
19     p_rghFinal
20     {
21         $p_rgh;
22         relTol           0;
23     }
24
25     "(U|h)"
26     {
27         solver          PBiCG;
28         preconditioner   DILU;
29         tolerance        1e-6;
30         relTol           0.1;
31     }
32
33     "(U|h)Final"
34     {
35         $U;
36         relTol           0;
37     }
38 }
39
40 PIMPLE
41 {
42     momentumPredictor yes;
43     nOuterCorrectors 20;
44     nCorrectors      2;
45     nNonOrthogonalCorrectors 1;
46     residualControl
47     {
48         "(U|h)"
49         {
50             tolerance 1e-4;
51             relTol     0;
52         }
53         p_rgh
54         {
55             tolerance 1e-4;
56             relTol     0;
57         }
58     }
59 }

```

### 3.2.3 Running the simulation in parallel

The *decomposeParDict* is the same as the previous part and in a similar manner the parallel execution is performed with the commands:

```
decomposePar -force
```

```
foamJob -screen -parallel buoyantPimpleFoam
```

And then, to leave it ready for the post-processing:

```
reconstructPar
```



### 3.2.4 Post-processing

The average Nusselt is compared with the one obtained with Morgan's correlation based on experimental data (as cited by S.K.S. Boetcher, 2014 [3]):

$$\overline{Nu}_D = 0.48 \cdot Ra_D^{(1/4)}$$

As shown in Table 7 there's good agreement between the simulation result and the correlation with only a difference of a 7.31%.

Simulation heat rate [W]	Simulation $\overline{Nu}_D$	Correlation $\overline{Nu}_D$	Simulation/Correlation [%]
209.67	9.9086	9.2328	7.31

Table 7: Comparison between the average Nusselt numbers from the simulation and Morgan's correlation.

Figure 29 displays the temperature distribution at different times. In a real case the rising air becomes turbulent at some point but since this is a laminar flow simulation it doesn't, yet the results relative to the heat transfer are good as it doesn't have a significant effect on the flow around the cylinder.

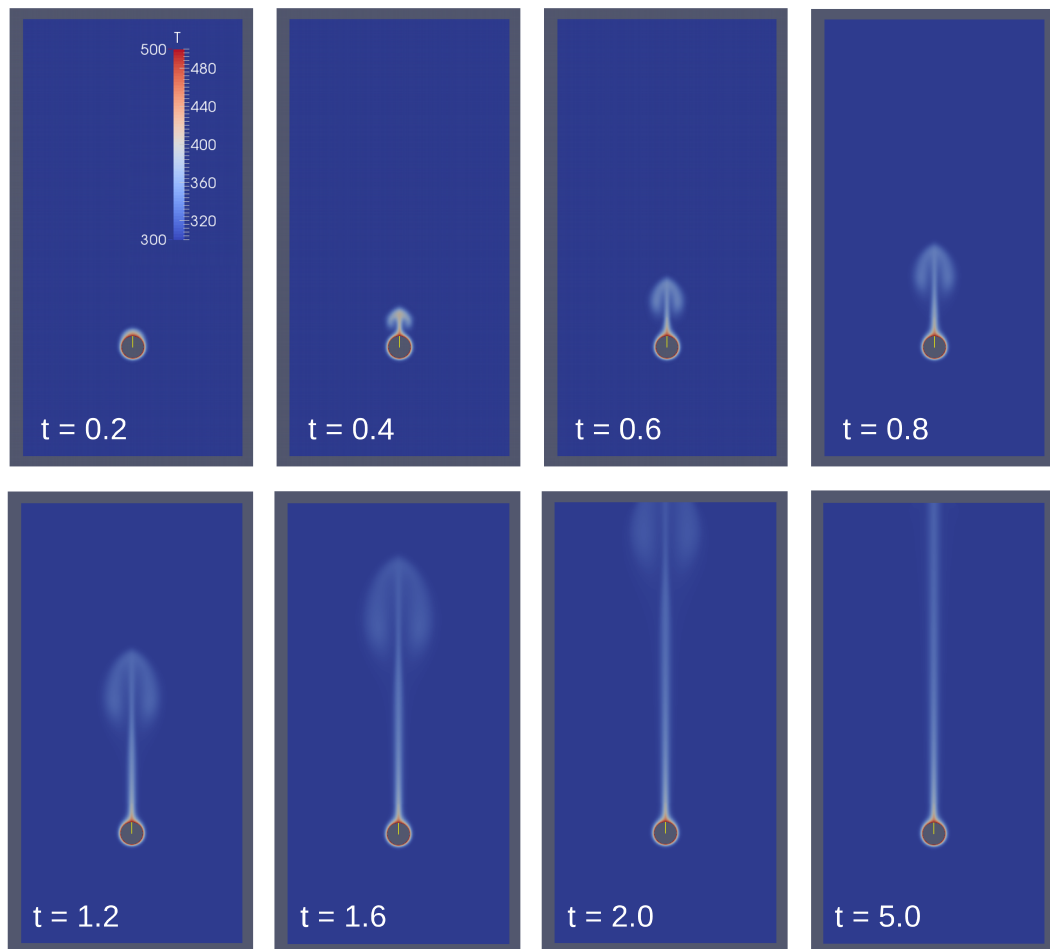


Figure 29: Temperature distribution at different times (same scale on all).

A proper reproduction of this turbulent transition would require a very expensive direct numerical simulation (DNS), with a grid fine enough to capture the eddies up to the Kolmogorov microscales, or modeling the phenomenon partially/entirely through a turbulence model (Large Eddy Simulation / Reynolds Averaged Simulation), which reduces the computational effort at the expense of some accuracy, but it is still unnecessary for a case like this.

Finally Figure 30 shows the streamlines at different times.

In order to visualize the streamlines with paraFoam first it's necessary to apply a *Slice* filter to cut a slice normal to the z-direction and then use the *Stream Tracer* filter on this *Slice*. Within *Stream Tracer* properties there's an option named *Seed Type*, here the user can select *High Resolution Line Source* to place a line and trace the streamlines crossing it. A more complete representation can be achieved by using several Stream Tracer filters and placing the lines conveniently.

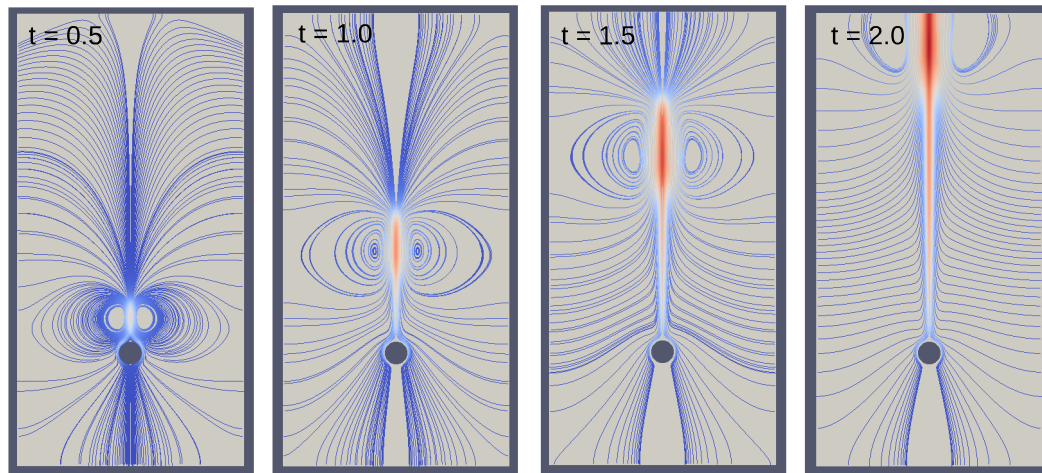


Figure 30: Streamlines at different times.

# Chapter 4 - Conjugate Heat Transfer

This chapter is the practical application of the two previous ones into a conjugate heat transfer problem involving solid and fluid regions using `chtMultiRegionSimpleFoam`. It also introduces a way to model variable thermo-physical properties on the flow.

## 4.1 Description of the case

The case consists on an horizontal wall composed of two materials A and B with different thermal conductivities (indicated in Table 8) with the top and bottom sides exposed to forced, horizontal, external flows of dry air at different temperatures (see Figure 31 for details). The left and right sides of the wall are considered adiabatic.

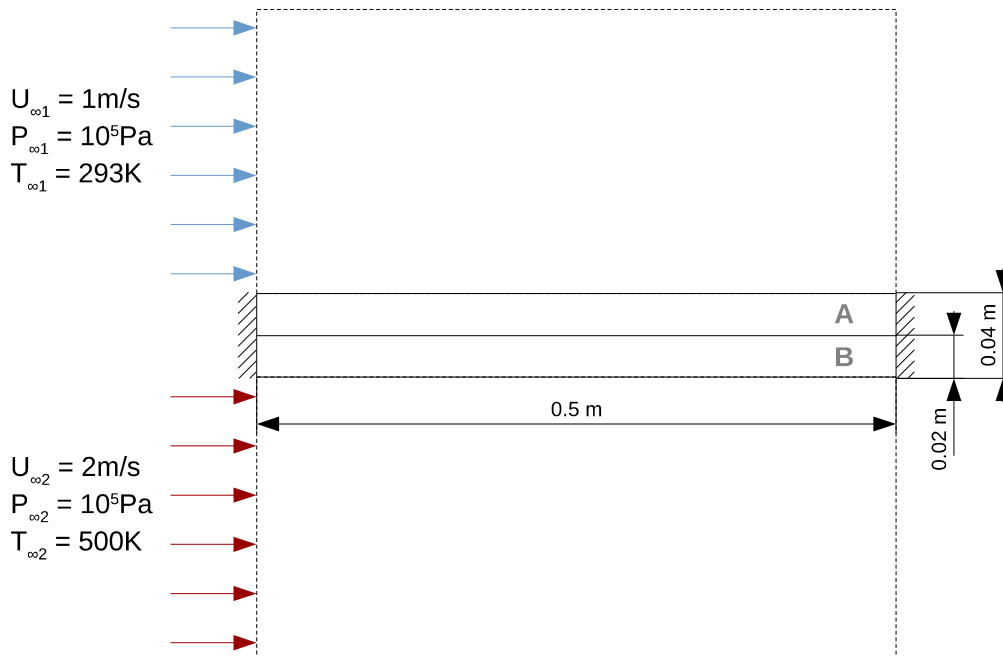


Figure 31: Schematic of the case.

Material	Thermal conductivity [W/(m <sup>2</sup> · K)]
A	1
B	200

Table 8: Thermal conductivities of the solid materials.

#### 4.1.1 Assumptions

- Steady-state conditions
- Bi-dimensional, compressible, laminar flow
- Newtonian fluid
- Perfect gas
- The thermo-physical properties of the fluids are functions of the temperature
- The thermal conductivities of the solids are constant and uniform
- No contact resistance between solids
- Negligible radiation effects

#### 4.1.2 Formulation

The formulation of the problem is the same seen on previous cases. On one side there are the conservation equations which, once simplified, are the same as in 3.1.1.2:

$$\nabla \cdot (\rho \vec{u}) = 0$$

$$\rho(\vec{u} \cdot \nabla \vec{u}) = -\nabla \cdot p + \nabla \cdot \vec{\tau} + \rho \cdot \vec{g}$$

$$\rho(\vec{u} \cdot \nabla h + \vec{u} \cdot \nabla e_c) = \frac{\partial p}{\partial t} + \nabla \cdot (\kappa \nabla T) + \nabla \cdot (\vec{\tau} \cdot \vec{u}) + \rho \vec{g} \cdot \vec{u}$$

And on the other side the heat equation which for this case is reduced to:

$$\nabla^2 T = 0$$

The solver solves each region separately according to the applicable equations and couples them with a boundary condition of equal heat flux through the surfaces of contact ( the `turbulentTemperatureCoupledBaffleMixed`).

As for the thermo-physical properties of air, now dependent on the temperature, they are modeled using the following expressions:

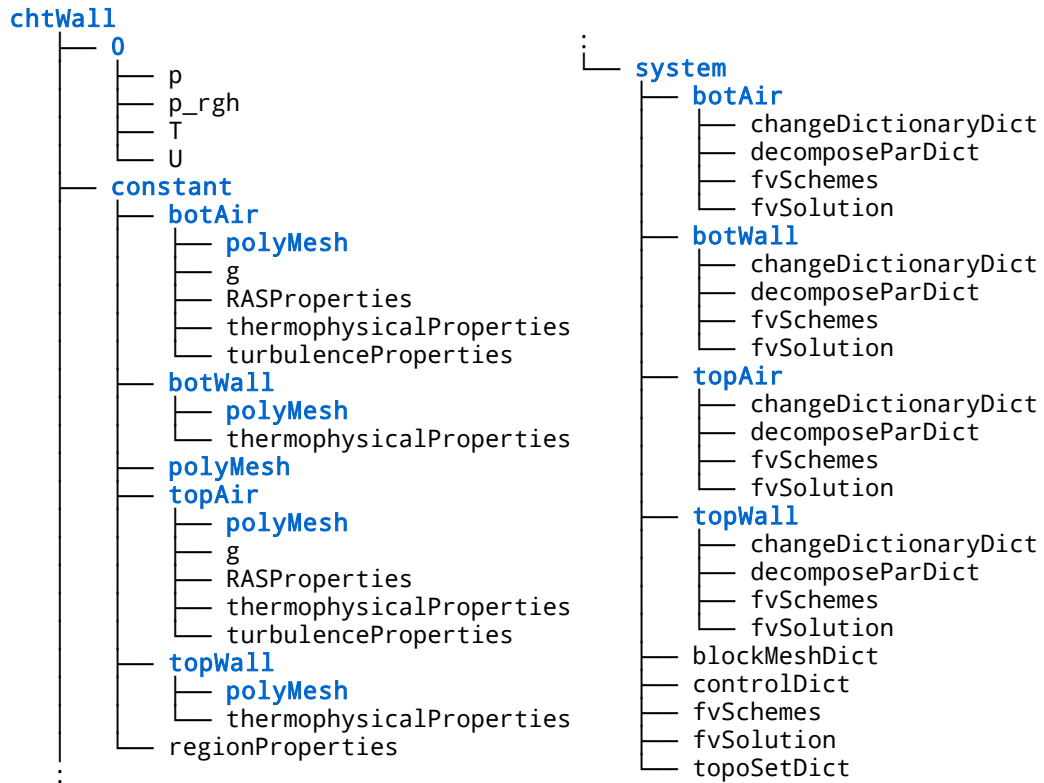
$$c_p = 1034.09 - 2.849 \cdot 10^{-1} T + 7.817 \cdot 10^{-4} T^2 - 4.971 \cdot 10^{-7} T^3 + 1.077 \cdot 10^{-10} T^4$$

$$\mu = \frac{1.458 \cdot 10^{-6} T^{-1.5}}{T + 110.4} \quad (\text{Sutherland's formula})$$

$$\kappa = \mu c_v \left( 1.32 + \frac{1.77 R_{air}}{c_v} \right) \quad (\text{modified Eucken's model})$$

## 4.2 Preprocessing

Structure of the case:



### 4.2.1 Mesh generation

The mesh is generated with *blockMesh* using the next *blockMeshDict*:

```

1  convertToMeters 1;
2
3  vertices
4  (
5      (0 -0.25 0)
6      (0.5 -0.25 0)
7      (0.5 0.25 0)
8      (0 0.25 0)
9      (0 -0.25 1)
10     (0.5 -0.25 1)
11     (0.5 0.25 1)
12     (0 0.25 1)
13 );
14
15 blocks
16 (
17     hex (0 1 2 3 4 5 6 7) (100 250 1)
18     simpleGrading
19     (5
20         (
21             (0.23 100 0.02)
22             (0.04 50 1)
23             (0.23 100 50)
24         )
25     1)
26 );
27
28 edges
  
```

```

29 (
30 );
31
32 boundary
33 (
34     maxY
35     {
36         type patch;
37         faces
38         (
39             (3 7 6 2)
40         );
41     }
42     minX
43     {
44         type patch;
45         faces
46         (
47             (0 4 7 3)
48         );
49     }
50     maxX
51     {
52         type patch;
53         faces
54         (
55             (2 6 5 1)
56         );
57     }
58     minY
59     {
60         type patch;
61         faces
62         (
63             (1 5 4 0)
64         );
65     }
66 );
67
68 mergePatchPairs
69 (
70 );
71
72 // *****

```

The approach is similar as the one used for the grid in 3.1.2.1 (convection over horizontal plate case): using a graded grid on the flow regions to achieve a finer mesh near the wall. This is achieved through the multi-grading feature of *blockMesh*, this feature is available since OpenFOAM v2.4 and allows the definition of multiple graded zones along a direction by replacing the corresponding expansion ratio. Each zone is defined by an array with three variables, the first one defines the fraction of the total length the zone occupies, the second the fraction of cells it has and the third specifies its grading.

In this *blockMeshDict* the expansion ratio corresponding to the y-direction has been replaced by:

```

20     (
21     (0.23 100 0.02)
22     (0.04 50 1)
23     (0.23 100 50)
24     (

```

This means the first 23cm of the height contains 100 cells with a grading of 1/50 (the mesh is refined towards the direction of y), the next 4cm (the wall) has 50 cells without grading and the remaining 23cm contains the rest of the cells with a grading of 50 (the

mesh is coarsened towards the direction of y).

*Note: Though the first two variables are fractions they are normalized automatically (i.e. in the example 0.23 actually means a fraction of  $0.23/[0.23+0.04+0.23]$  of the total height) so they can be expressed the way the user feels more convenient.*

In addition a simple grading is used for the x-direction too because of the greater gradients expected towards the inlet as the boundary layers start developing. Figure 32 and Figure 33 show the resulting mesh.

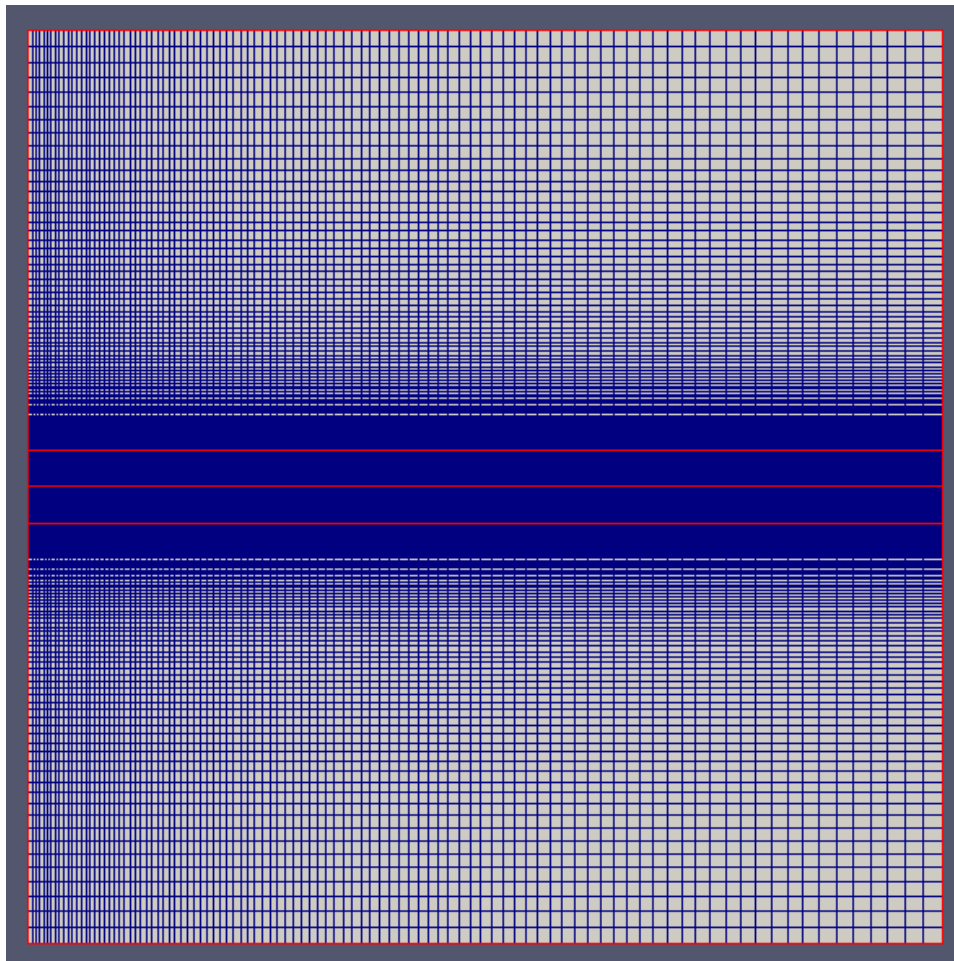


Figure 32: General view of the mesh (red lines differentiate the regions).

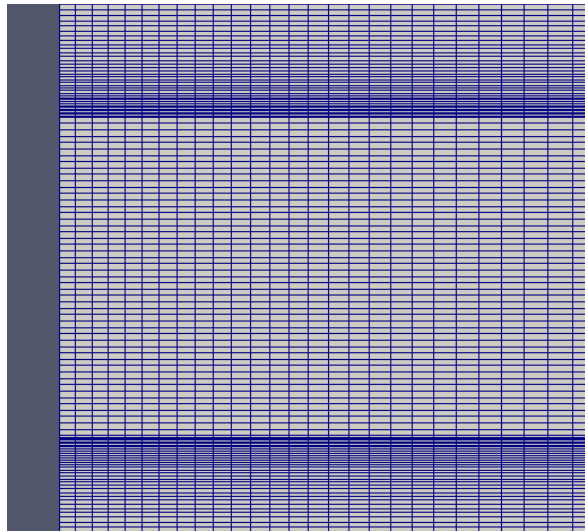


Figure 33: Detail view of the mesh around the wall.

Finally the following *topoSetDict* sets the *cellZones* of the four regions into which the *splitMeshRegions* tool will divide the mesh (from top to bottom: *topAir*, *topWall*, *botWall* and *botAir*):

```

1  actions
2  (
3
4    // topAir
5    {
6      name    topAir; //name of the set
7      type    cellSet;
8      action  new; //create a new set
9      source  boxToCell; //use a selection box
10     sourceInfo
11     {
12       box (0 0.02 0)(1 0.25 1); //box corners
13     }
14   }
15   {
16     name    topAir;
17     type    cellZoneSet;
18     action  new;
19     source  setToCellZone;
20     sourceInfo
21     {
22       set topAir;
23     }
24   }
25
26   // botAir
27   {
28     name    botAir;
29     type    cellSet;
30     action  new;
31     source  boxToCell;
32     sourceInfo
33     {
34       box (0 -0.25 0)(1 -0.02 1);
35     }
36   }
37   {
38     name    botAir;
39     type    cellZoneSet;
40     action  new;

```



```

41         source setToCellZone;
42         sourceInfo
43         {
44             set botAir;
45         }
46     }
47
48     // topWall
49     {
50         name    topWall;
51         type    cellSet;
52         action  new;
53         source  boxToCell;
54         sourceInfo
55         {
56             box (0 0 0)(1 0.02 1);
57         }
58     }
59     {
60         name    topWall;
61         type    cellZoneSet;
62         action  new;
63         source  setToCellZone;
64         sourceInfo
65         {
66             set topWall;
67         }
68     }
69     // botWall
70     {
71         name    botWall;
72         type    cellSet;
73         action  new;
74         source  boxToCell;
75         sourceInfo
76         {
77             box (0 -0.02 0)(1 0 1);
78         }
79     }
80     {
81         name    botWall;
82         type    cellZoneSet;
83         action  new;
84         source  setToCellZone;
85         sourceInfo
86         {
87             set botWall;
88         }
89     }
90 );
91
92 // *****

```

## 4.2.2 Boundary conditions

The boundary conditions are specified almost entirely within the *changeDictionaryDict* of each region. For this reason on all the files in the *0* directory, *p*, *p\_rgh*, *T* and *U*; the *boundaryField* is left as:

```

1 boundaryField
2 {
3     ".*"
4     {
5         type    calculated;
6         value    $internalField;
7     }
8
9     defaultFaces
10    {

```

```

11         type          empty;
12     }
13 }
14
15
16 // *****

```

This serves as a placeholder for the *splitMeshRegions* tool so after the mesh is divided the contents of the boundary files of each region can be replaced with the actual conditions using the *changeDictionary* tool. The associated dictionaries are exposed below. Because of this methodology, after splitting the mesh the newly generated directories of the solid regions also have the *U* and *p\_rgh* files which have to be deleted, the solid regions shouldn't have anything other than *T* and *p*.

*/botAir/changeDictionaryDict:*

```

1 dictionaryReplacement
2 {
3     T
4     {
5         internalField    uniform 500;
6         boundaryField
7         {
8             "m.*" //any patch starting with m
9             {
10                 type          inletOutlet;
11                 inletValue    uniform 500;
12                 value         uniform 500;
13             }
14             botAir_to_botWall
15             {
16                 type
compressible::turbulentTemperatureCoupledBaffleMixed;
17                 Tnbr          T;
18                 kappa          fluidThermo;
19                 kappaName      none;
20                 value          uniform 500;
21             }
22         }
23     }
24 }
25
26 U
27 {
28     internalField    uniform (2 0 0);
29     boundaryField
30     {
31         minX
32         {
33             type          fixedValue;
34             value          $internalField;
35         }
36         maxX
37         {
38             type          inletOutlet;
39             inletValue    uniform (0 0 0);
40             value          $internalField;
41         }
42         minY
43         {
44             type          zeroGradient;
45             value          $internalField;
46         }
47         botAir_to_botWall
48         {
49             type          fixedValue;

```

```

51             value          uniform (0 0 0);
52         }
53     }
54 }
55 p_rgh
56 {
57     internalField    uniform 1e5;
58     boundaryField
59     {
60         minX
61         {
62             type          fixedFluxPressure;
63             value          $internalField;
64         }
65         maxX
66         {
67             type          fixedFluxPressure;
68             value          $internalField;
69         }
70         minY
71         {
72             type          fixedValue;
73             value          $internalField;
74         }
75         botAir_to_botWall
76         {
77             type          fixedFluxPressure;
78             value          $internalField;
79         }
80     }
81 }
82
83 }
84
85 // ***** //

```

*/topAir/changeDictionaryDict:*

```

1  dictionaryReplacement
2  {
3      T
4      {
5          internalField    uniform 293;
6          boundaryField
7          {
8              "m.*"
9              {
10                 type          inletOutlet;
11                 inletValue    uniform 293;
12                 value          uniform 293;
13             }
14             topAir_to_topWall
15             {
16                 type
compressible::turbulentTemperatureCoupledBaffleMixed;
17                 Tnbr          T;
18                 kappa          fluidThermo;
19                 kappaName      none;
20                 value          uniform 293;
21             }
22         }
23     }
24 }
25
26 U
27 {
28     internalField    uniform (1 0 0);
29     boundaryField
30     {
31         minX
32         {

```

```

33             type          fixedValue;
34             value          $internalField;
35         }
36         maxX
37         {
38             type          inletOutlet;
39             inletValue     uniform (0 0 0);
40             value          $internalField;
41         }
42         maxY
43         {
44             type          zeroGradient;
45             value          $internalField;
46         }
47
48         topAir_to_topWall
49         {
50             type          fixedValue;
51             value          uniform (0 0 0);
52         }
53     }
54 }
55 p_rgh
56 {
57     internalField    uniform 1e5;
58     boundaryField
59     {
60         minX
61         {
62             type          fixedFluxPressure;
63             value          $internalField;
64         }
65         maxX
66         {
67             type          fixedFluxPressure;
68             value          $internalField;
69         }
70         maxY
71         {
72             type          fixedValue;
73             value          $internalField;
74         }
75         topAir_to_topWall
76         {
77             type          fixedFluxPressure;
78             value          $internalField;
79         }
80     }
81 }
82
83 }
84
85 // *****

```

/botAir/changeDictionaryDict:

```

1 dictionaryReplacement
2 {
3     T
4     {
5         internalField    uniform 400;
6         boundaryField
7         {
8             minX
9             {
10                type          zeroGradient;
11                value          uniform 400;
12            }
13            maxX
14            {
15                type          zeroGradient;

```

```

16             value          uniform 400;
17         }
18     botWall_to_topwall
19     {
20         type
compressible::turbulentTemperatureCoupledBaffleMixed;
21         Tnbr              T;
22         kappa              solidThermo;
23         kappaName          none;
24         value              uniform 400;
25     }
26     botWall_to_botAir
27     {
28         type
compressible::turbulentTemperatureCoupledBaffleMixed;
29         Tnbr              T;
30         kappa              solidThermo;
31         kappaName          none;
32         value              uniform 500;
33     }
34 }
35 }
36
37 }
38
39 // ***** //
```

*/botAir/changeDictionaryDict:*

```

1 dictionaryReplacement
2 {
3     T
4     {
5         internalField    uniform 400;
6         boundaryField
7         {
8             minX
9             {
10                 type          zeroGradient;
11                 value          uniform 400;
12             }
13             maxX
14             {
15                 type          zeroGradient;
16                 value          uniform 400;
17             }
18             topWall_to_topAir
19             {
20                 type
compressible::turbulentTemperatureCoupledBaffleMixed;
21                 Tnbr          T;
22                 kappa          solidThermo;
23                 kappaName      none;
24                 value          uniform 293;
25             }
26             topWall_to_botWall
27             {
28                 type
compressible::turbulentTemperatureCoupledBaffleMixed;
29                 Tnbr          T;
30                 kappa          solidThermo;
31                 kappaName      none;
32                 value          uniform 400;
33             }
34         }
35     }
36 }
37
38 // ***** //
```

The specific conditions combine what's seen in the chapters 2 and 3. Initially a `fixedPressure` condition was used on the outlets but it was observed this can cause convergence issues for low velocity flows and the `fixedFluxPressure` condition gives better results.

### 4.2.3 Properties

This chapter introduces some guidelines on the specification of temperature-dependent thermo-physical properties. To model that, this *thermophysicalProperties* dictionary is used for both the *topAir* and *botAir* regions:

```

1  thermoType
2  {
3      type            heRhoThermo;
4      mixture         pureMixture;
5      transport       sutherland;
6      thermo          hPolynomial;
7      equationOfState perfectGas;
8      specie          specie;
9      energy          sensibleEnthalpy;
10 }
11
12 mixture
13 {
14     specie
15     {
16         nMoles        1;
17         molWeight     28.9;
18     }
19     thermodynamics
20     {
21         CpCoeffs<8>   ( 1034.09 -2.849e-1 7.817e-4 -4.971e-7 1.077e-10 0 0 0);
22         Hf            0;
23         Sf            0;
24     }
25     transport
26     {
27         AS            1.458e-06;
28         TS            110.4;
29     }
30 }
31
32
33 // ***** //
```

First, within `thermoType`, the keywords `transport sutherland` and `thermo hPolynomial` enables the use of the Sutherland/Eucken models and polynomial expressions for the heat capacity.

With this, given a polynomial expression:

$$c_p = \sum_{i=0}^7 a_i T^i$$

The eight  $a_i$  coefficients are introduced in the form of an ordered array after `CpCoeffs<8>` (line 21).

And given the relation:

$$\mu = \frac{A_s \cdot T^{-1.5}}{T + T_s}$$

The  $A_s$  and  $T_s$  coefficients are specified after the keywords  $A_s$  and  $T_s$  (lines 27, 28).

With these and the molar weight (`molWeight`) all the terms of the modified Eucken's expression are determined so it doesn't need a particular entry.

This particular combination of models isn't part of the default pre-compiled set so it needs to be compiled or otherwise it won't work. To do so it's only necessary to add the following lines of code to the file `/openfoam240/src/thermophysicalModels/basic/rhoThermo/rhoThermos.C` after the last `makeThermo`:

```
makeThermo
(
    rhoThermo,
    heRhoThermo,
    pureMixture,
    sutherlandTransport,
    sensibleEnthalpy,
    hPolynomialThermo,
    perfectGas,
    specie
);
```

And next open the terminal and run this two commands from within that same directory (the directory were `rhoThermos.C` is):

```
sudo bash
wmake libso
```

Now that combination of models can be used.

The rest of properties files are as usual. *RASProperties* and *turbulenceProperties* are set in laminar mode, the *g* files specify a downwards acceleration of 9,81m/s<sup>2</sup> and the *thermophysicalProperties* of the solids simply specify the corresponding thermal conductivities after the `kappa` keyword (remember since they're solids under steady-state conditions only the other values aren't meaningful).

Finally *regionProperties* should look as follows:

```
1 regions
2 (
3     fluid    (topAir botAir)
4     solid    (topWall botWall)
5 );
6
7 // ***** //
```

## 4.2.4 Control, solution and schemes

*controlDict:*

```

1  application      chtMultiRegionSimpleFoam;
2
3  startFrom        latestTime;
4
5  startTime        0;
6
7  stopAt           endTime;
8
9  endTime          6500;
10
11 deltaT           1;
12
13 writeControl      timeStep;
14
15 writeInterval     500;
16
17 purgeWrite        0;
18
19 writeFormat        ascii;
20
21 writePrecision     9;
22
23 writeCompression  off;
24
25 timeFormat         general;
26
27 timePrecision      6;
28
29 runTimeModifiable true;
30
31
32 // ***** //
```

*botAir and topAir fvSolution:*

```

1  solvers
2  {
3      p_rgh
4      {
5          solver          PCG;
6          preconditioner   DIC;
7          tolerance        1e-9;
8          relTol           0.01;
9      }
10
11      "(U|h)"
12      {
13          solver          PBiCG;
14          preconditioner   DILU;
15          tolerance        1e-9;
16          relTol           0.1;
17      }
18  }
19
20 SIMPLE
21 {
22     momentumPredictor no;
23     nNonOrthogonalCorrectors 0;
24     pRefCell            0;
25     pRefValue            100000;
26     rhoMin               rhoMin [1 -3 0 0 0] 0.2;
27     rhoMax               rhoMax [1 -3 0 0 0] 2;
28
29 }
30
31 relaxationFactors
32 {
33     rho                  1.0;
34     p_rgh                 0.7;
35     U                     0.7;
```



```

36     h                0.7;
37 }
38
39 // ***** //

```

*botAir* and *topAir* fvSchemes:

```

1  ddtSchemes
2  {
3      default          steadyState;
4  }
5
6  gradSchemes
7  {
8      default          Gauss linear;
9  }
10
11 divSchemes
12 {
13     default            bounded Gauss upwind;
14     div((muEff*dev2(T(grad(U)))) Gauss linear;
15 }
16
17 laplacianSchemes
18 {
19     default            Gauss linear uncorrected;
20 }
21
22 interpolationSchemes
23 {
24     default            linear;
25 }
26
27 snGradSchemes
28 {
29     default            uncorrected;
30 }
31
32 fluxRequired
33 {
34     default            no;
35     p_rgh;
36 }
37
38
39 // ***** //

```

*botWall* and *topWall* fvSolution:

```

1  solvers
2  {
3      h
4      {
5          solver          PCG;
6          preconditioner   DIC;
7          tolerance       1e-9;
8          relTol           0.1;
9      }
10 }
11
12 SIMPLE
13 {
14     nNonOrthogonalCorrectors 0;
15 }
16
17 relaxationFactors
18 {
19     h                1;
20 }

```

```
21
22
23 // ***** //
```

*botWall* and *topWall* *fvSchemes*:

```
1 ddtSchemes
2 {
3     default      steadyState;
4 }
5
6 gradSchemes
7 {
8     default      Gauss linear;
9 }
10
11 divSchemes
12 {
13     default      none;
14 }
15
16 laplacianSchemes
17 {
18     default      none;
19     laplacian(alpha,h) Gauss linear uncorrected;
20 }
21
22 interpolationSchemes
23 {
24     default      linear;
25 }
26
27 snGradSchemes
28 {
29     default      uncorrected;
30 }
31
32 fluxRequired
33 {
34     default      no;
35 }
36
37 // ***** //
```

## 4.3 Running the simulation in parallel

As the cases grow in complexity taking advantage of the linux bash scripting becomes more useful. The post-preprocessing phase can be completed with the next script:

```
1 #!/bin/bash
2
3 blockMesh
4 topoSet
5 splitMeshRegions -cellZones -overwrite
6
7 rm ./0/topWall/{p_rgh,U}
8 rm ./0/botWall/{p_rgh,U}
9
10 for i in topAir botAir topWall botWall
11 do
12     changeDictionary -region $i > log.changeDictionary.$i 2>&1
13 done
```

And this one to run the simulation in parallel:

```
1  #!/bin/sh
2
3  decomposePar -force -allRegions
4  foamJob -screen -parallel chtMultiRegionSimpleFoam
```

These scripts are saved in the case directory under the name the user prefers, e.g. *Prep* and *Run*, so each phase can be initiated by only typing in the terminal:

**bash Prep**

**bash Run**

Also note that to run the simulation in parallel a *decomposeParDict* file has to be present not only in the system directory but also in each of the region folders inside. The file can be the same for all the locations:

```
1  numberOfSubdomains 4;
2
3  method          simple;
4
5  simpleCoeffs
6  {
7      n              ( 2 2 1 );
8      delta          0.001;
9  }
10
11 distributed      no;
12
13 roots            ( );
14
15
16 // ***** //
```

## 4.4 Post-processing

Table 9 shows the global heat rates through the patches of contact between regions, obtained using the *wallHeatFlux* tool on each region. The differences are small, indicating a good level of convergence, the residuals of the last iteration of the solver are very small as well so the slight discrepancies could be due to discretization errors.

Patch (region)	Heat rate [W]
botAir_to_botWall (botAir)	-333.61
botWall_to_botAir (botWall)	333.49
botWall_to_topWall (botWall)	-333.50
topWall_to_botWall (topWall)	333.50
topWall_to_topAir (topWall)	-333.50
topAir_to_topWall (topWair)	333.44

Table 9: Heat rates on the patches of contact. Positive values for an entering flux.

To end, some more results are shown with the next figures.

Temperature distribution with a custom coloring to better appreciate the gradients within the wall:

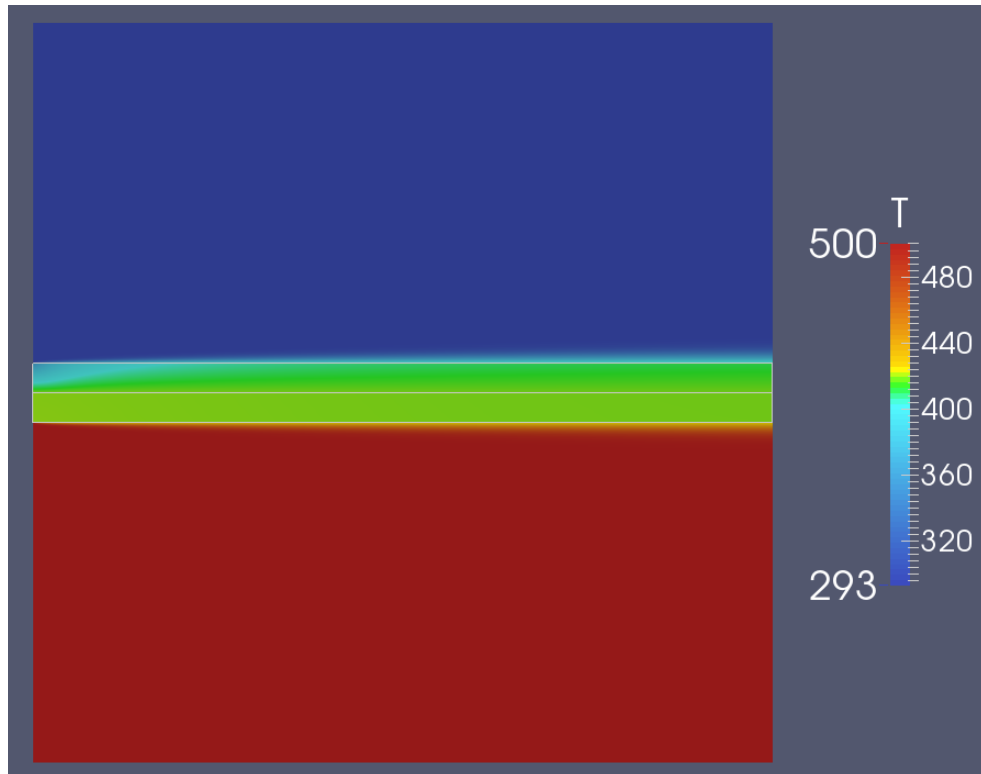


Figure 34: Temperature distribution.

Temperature profile near the wall at  $x=0.4m$ . The result is as expected, the flows near the wall form a thermal boundary layer and the wall has differentiated temperature gradients due to the different conductivities:

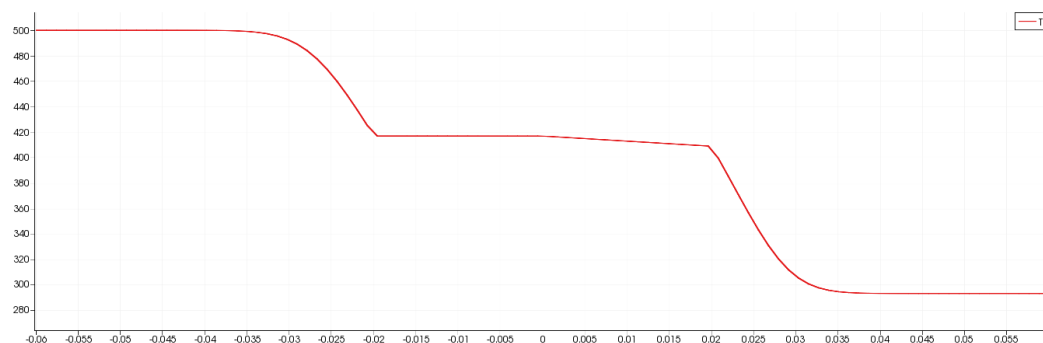


Figure 35: Temperature [K] vs.  $y$  [m] at  $x = 0.4m$

# Chapter 5 - Radiation

To conclude this guide the fifth chapter explains the implementation of surface-to-surface radiation with non-participating media. The used solvers are `buoyantSimpleFoam` and `chtMulti-RegionSimpleFoam` which have already been exposed in previous chapters so this one focuses on the radiation part.

Part B also explains the introduction of heat sources and develops a complete case of conduction, convection and radiation with heat sources.

## 5.1 Part A: Convection + Radiation

### 5.1.1 Description of the case

The case consists of a square, bi-dimensional enclosure filled with dry air whose top and bottom walls are adiabatic and the side walls are isothermal, with the left one having a higher temperature than the right. All the walls have an emissivity  $\varepsilon = 0.8$ . The rest of details are shown in Figure 36. This case is based on the numerical study of Wang *et al.* (2006) [11], which studies this problem under the Boussinesq approximation.

The thermo-physical properties are defined as the properties of the dry-air evaluated at  $T_0 = 293.5\text{K}$  (Table 10).

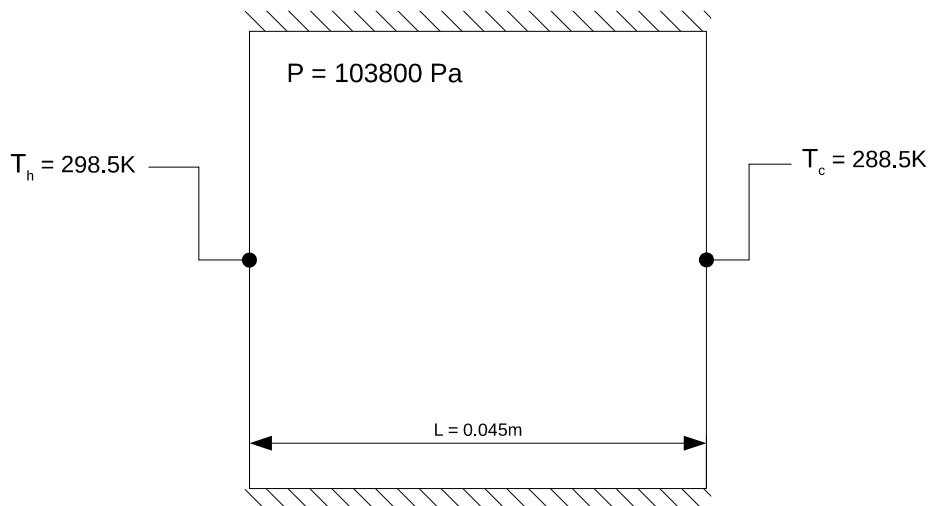


Figure 36: Diagram of the case.

$c_p$ [J/(kg·K)]	$\mu$ [ $10^{-5}$ kg/(m·s)]	$\kappa$ [W/(m·K)]	$Pr$
1011	1.8151	0.02576	0.7124

Table 10: Thermo-physical properties of the fluid.

### 5.1.1.1 Assumptions

- Steady-state conditions.
- Bi-dimensional, compressible, laminar flow
- Newtonian fluid
- Perfect gas
- Constant thermo-physical properties
- Surface-to-surface radiation with non-participating medium
- The internal walls are gray, diffuse, opaque surfaces with a constant, uniform emissivity

### 5.1.2 Formulation

This case has the same governing equations as 3.1.1.2 with the addition of a radiation model. The Rayleigh number is:

$$Ra_L = \frac{g\beta(T_h - T_c)L^3}{\nu\alpha} = 10^5$$

Because the medium is non-participating the radiation only affects the boundaries through the surface-to-surface radiation exchange and since two of the walls haven't a fixed temperature there's an interaction with the convection mode.

The radiation model of the simulation is based on the “radiosity method”. The method relies on the last two of the listed assumptions which allow the radiosity (radiant energy abandoning a surface, represented as  $J$ ) and the irradiation (incident radiant energy, represented as  $G$ ) of a surface  $k$  to be calculated as:

$$J_k = \varepsilon_k \sigma T^4 + (1 - \varepsilon) G_k$$

$$G_k = \sum_{i=1}^N F_{ki} J_i$$

Where the view factors,  $F_{ki}$ , depend on the geometry and are defined as:

$$F_{ki} = \frac{1}{A_k} \int_{A_k} \int_{A_i} \frac{\cos\theta_k \cos\theta_i}{\pi S^2} dA_k dA_i$$

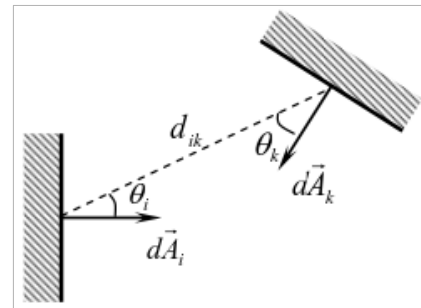


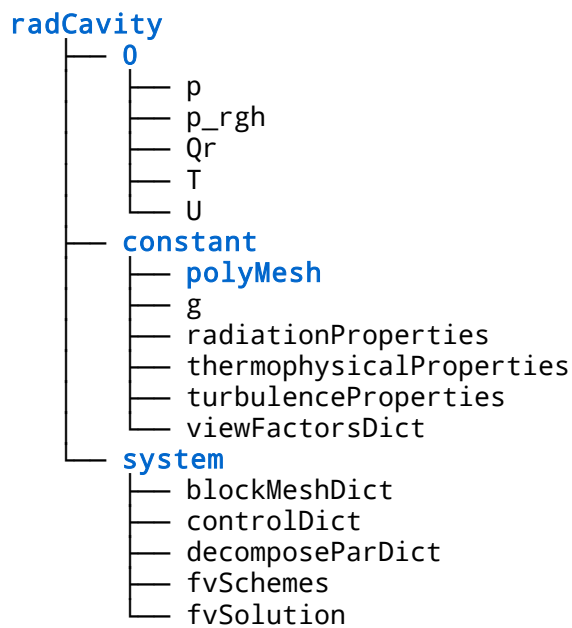
Figure 37: Differential areas for view factors calculation [13].

Finally the definition of net radiative heat flux depends on the sign criteria. OpenFOAM uses positive values for a flux entering the surface, therefore:

$$q_{\text{rad},k} = G_k - J_k$$

### 5.1.3 Preprocessing

Structure of the case:



#### 5.1.3.1 Mesh Generation

A simple 120x120 grid is used for this case. The mesh is generated with *blockMesh* as usual, using the next *blockMeshDict*:

```

1  convertToMeters 1;
2
3  vertices
4  (
5      (0 0 0)
6      (0.045 0 0)
7      (0.045 0.045 0)
8      (0 0.045 0)
9      (0 0 1)
10     (0.045 0 1)
11     (0.045 0.045 1)
12     (0 0.045 1)
13 );
14
15 blocks
16 (
17     hex (0 1 2 3 4 5 6 7) (120 120 1) simpleGrading (1 1 1)
18 );
19
20 edges
21 (
22 );
  
```

```

23
24 boundary
25 (
26     maxY
27     {
28         type wall;
29         faces
30         (
31             (3 7 6 2)
32         );
33     }
34     minX
35     {
36         type wall;
37         faces
38         (
39             (0 4 7 3)
40         );
41     }
42     maxX
43     {
44         type wall;
45         faces
46         (
47             (2 6 5 1)
48         );
49     }
50     minY
51     {
52         type wall;
53         faces
54         (
55             (1 5 4 0)
56         );
57     }
58 );
59
60 mergePatchPairs
61 (
62 );
63
64 // ***** //
```

### 5.1.3.2 Boundary conditions

The inclusion of the radiation in the problem implies a new file named *Qr* which is the field corresponding to the radiative heat flux and is used to define the related conditions.

*Qr*:

```

1 dimensions      [1 0 -3 0 0 0 0];
2
3 internalField    uniform 0;
4
5 boundaryField
6 {
7     minX
8     {
9         type                greyDiffusiveRadiationViewFactor;
10        emissivityMode       lookup;
11        Qro                   uniform 0;
12        emissivity            uniform 0.8;
13        value                 uniform 0;
14    }
15    maxX
16    {
17        type                greyDiffusiveRadiationViewFactor;
18        emissivityMode       lookup;
19        Qro                   uniform 0;
```



```

20             emissivity      uniform 0.8;
21             value           uniform 0;
22         }
23     minY
24     {
25         type                greyDiffusiveRadiationViewFactor;
26         emissivityMode      lookup;
27         Qro                  uniform 0;
28         emissivity          uniform 0.8;
29         value                uniform 0;
30     }
31     maxY
32     {
33         type                greyDiffusiveRadiationViewFactor;
34         emissivityMode      lookup;
35         Qro                  uniform 0;
36         emissivity          uniform 0.8;
37         value                uniform 0;
38     }
39     defaultFaces
40     {
41         type                empty;
42     }
43 }
44
45 // ***** //

```

The condition type associated with the radiosity method is the `greyDiffusiveRadiationViewFactor` and hence it has to be used on every patch. The `emissivityMode` is set to either `lookup` for a direct specification of the emissivity of the wall or to `solidRadiation` to get the value from the properties of the solid region which only applies to multi-region problems. This condition also requires the definition of the external radiative heat flux, `Qro`, which in this case is 0 on all the patches.

*T:*

```

1  dimensions      [0 0 0 1 0 0 0];
2
3  internalField   uniform 293.5;
4
5  boundaryField
6  {
7      minX
8      {
9          type      fixedValue;
10         value     uniform 298.5;
11     }
12     maxX
13     {
14         type      fixedValue;
15         value     uniform 288.5;
16     }
17     minY
18     {
19         type      compressible::turbulentHeatFluxTemperature;
20         heatSource flux; // power [W]; flux [W/m2]
21         q          uniform 0; // heat power or flux
22         kappaName  none;
23         kappa      fluidThermo; // obtains kappa from thermo model
24         Qr         Qr; // name of the radiative flux
25         value      $internalField; // initial temperature value
26     }
27     maxY
28     {
29         type      compressible::turbulentHeatFluxTemperature;
30         heatSource flux;
31         q          uniform 0;

```

```

32         kappaName      none;
33         kappa           fluidThermo;
34         Qr              $internalField;
35         value            $internalField;
36     }
37     defaultFaces
38     {
39         type             empty;
40     }
41 }
42 }
43
44 // *****

```

The  $T$  file also use a new type of condition required to satisfy the restriction the adiabatic walls impose on the internal faces which has the form:

$$-q_{rad} + q_{conv,in} = -q_{rad} \pm \kappa (\nabla T) = 0$$

i.e. the sum of the radiative flux leaving the internal face (therefore entering the domain) and the inwards convective flux equals 0.

Consequently `turbulentHeatFluxTemperature` is the proper type for these adiabatic walls because it allows the definition of the total entering heat flux while taking into account the radiative flux, respecting the aforementioned restriction.

The rest of condition files doesn't need any particular commentary.

$U$ :

```

1  dimensions      [0 1 -1 0 0 0 0];
2
3  internalField    uniform (0 0 0);
4
5  boundaryField
6  {
7      "."
8      {
9          type      fixedValue;
10         value      uniform (0 0 0);
11     }
12     defaultFaces
13     {
14         type      empty;
15     }
16 }
17
18
19 // *****

```

$p$ :

```

1  dimensions      [1 -1 -2 0 0 0 0];
2
3  internalField    uniform 103800;
4
5  boundaryField
6  {
7      "."
8      {
9          type      calculated;
10         value      $internalField;
11     }

```

```

12
13     defaultFaces
14     {
15         type            empty;
16     }
17 }
18
19
20 // ***** //

```

*p\_rgh:*

```

1  dimensions      [1 -1 -2 0 0 0 0];
2
3  internalField    uniform 103800;
4
5  boundaryField
6  {
7      "."
8      {
9          type            fixedFluxPressure;
10         value            $internalField;
11     }
12     defaultFaces
13     {
14         type            empty;
15     }
16 }
17
18
19 // ***** //

```

### 5.1.3.3 Properties

Another two new files related with the radiation modeling are located in the *constant* directory: *radiationProperties* and *viewFactorsDict*.

*radiationProperties* in this case is used only to define the radiation model as the medium doesn't participate with the radiation and the related parameters are defined through the boundary conditions. The *viewFactor* model is the model corresponding to the described radiosity method. Other possible models which won't be described in this work are the P1 (for optically thick media) or the fvDOM (finite volume discrete ordinates model, the most versatile and computationally expensive of the three).

```

1  radiation        on;
2
3  radiationModel    viewFactor;
4
5  viewFactorCoeffs
6  {
7      smoothing true; //Smooth view factor matrix (use when in a close surface
8                      //to force Sum(Fij = 1)
9      constantEmissivity true; //constant emissivity on surfaces.
10 }
11
12 // Number of flow iterations per radiation iteration
13 solverFreq 3;
14
15 absorptionEmissionModel none;
16
17
18 scatterModel      none;
19

```

```
20 sootModel          none;
21
22 // ***** //
```

The *viewFactorsDict* is a dictionary related with the generation of the view factors. This file requires the definition of two parameters, *nFacesInCoarsestLevel* and *featureAngle*, for every patch (more on that later).

```
1  writeViewFactorMatrix    true;
2  writeFacesAgglomeration  true;
3  writePatchViewFactors    false;
4
5  minX
6  {
7      nFacesInCoarsestLevel    15;
8      featureAngle              10;
9  }
10
11  maxX
12  {
13      nFacesInCoarsestLevel    15;
14      featureAngle              10;
15  }
16
17  minY
18  {
19      nFacesInCoarsestLevel    15;
20      featureAngle              10;
21  }
22
23  maxY
24  {
25      nFacesInCoarsestLevel    15;
26      featureAngle              10;
27  }
28
29
30 // ***** //
```

Now the view factors, necessary for the simulation, can be generated by executing the commands:

```
faceAgglomerate
viewFactorsGen
```

The best values for the parameters of the *viewFactorsDict* depend on the geometry and there isn't a general rule to set them, the recommendation is to test and compare a few different values. Some criteria to determine when they are good can be checking the *viewFactorsField* (which appears in the 0 folder after running *viewFactorsGen*) is close to the unity on the boundary elements, or to run a few iterations to make sure the net radiation fluxes are consistent with the physics.

The rest of files are set as in previous chapters.

### 5.1.3.4 Control, solution and schemes

*controlDict:*

```

1  application      buoyantSimpleFoam;
2
3  startFrom        latestTime;
4
5  startTime        0;
6
7  stopAt           endTime;
8
9  endTime          5000;
10
11 deltaT           1;
12
13 writeControl      timeStep;
14
15 writeInterval     500;
16
17 purgeWrite        0;
18
19 writeFormat       ascii;
20
21 writePrecision    9;
22
23 writeCompression  off;
24
25 timeFormat        general;
26
27 timePrecision     6;
28
29 runTimeModifiable true;
30
31
32 // ***** //
```

*fvSolution:*

```

1  solvers
2  {
3      rho
4      {
5          solver      PCG;
6          preconditioner DIC;
7          tolerance    1e-7;
8          relTol       0.1;
9      }
10
11     p_rgh
12     {
13         solver      PCG;
14         preconditioner DIC;
15         tolerance    1e-7;
16         relTol       0.1;
17     }
18
19     "(U|h)"
20     {
21         solver      PBiCG;
22         preconditioner DILU;
23         tolerance    1e-7;
24         relTol       0.1;
25     }
26
27 }
28
29 SIMPLE
30 {
```

```

32     momentumPredictor off;
33     nNonOrthogonalCorrectors 0;
34     pRefCell      0;
35     pRefValue     0;
36 }
37
38 relaxationFactors
39 {
40     fields
41     {
42         rho      1.0;
43         p_rgh    0.7;
44     }
45     equations
46     {
47         U      0.7;
48         h      0.7;
49         Qr     0.7;
50     }
51 }
52
53 // ***** //
```

### *fvSchemes:*

```

1  ddtSchemes
2  {
3      default      steadyState;
4  }
5
6  gradSchemes
7  {
8      default      Gauss linear;
9  }
10
11 divSchemes
12 {
13     default      none;
14     div(phi,U)    bounded Gauss upwind;
15     div(phi,K)    bounded Gauss upwind;
16     div(phi,h)    bounded Gauss upwind;
17     div((muEff*dev2(T(grad(U)))) Gauss linear;
18 }
19
20 laplacianSchemes
21 {
22     default      Gauss linear uncorrected;
23 }
24
25 interpolationSchemes
26 {
27     default      linear;
28 }
29
30 snGradSchemes
31 {
32     default      uncorrected;
33 }
34
35 fluxRequired
36 {
37     default      no;
38     p_rgh;
39 }
40
41 // ***** //
```

### 5.1.4 Running the simulation in parallel

The aforementioned `faceAgglomerate` and `viewFactorsGen` commands correspond to the serial execution, to run the simulation in parallel the next commands have to be used after preparing the preprocessing files and generating the mesh:

```

decomposePar -force
mpirun -np 4 faceAgglomerate -parallel
mpirun -np 4 viewFactorsGen -parallel
foamJob -screen -parallel buoyantSimpleFoam
  
```

### 5.1.5 Post-processing

This time the global heat rates will be analyzed with *paraFoam* and compared with the results of Wang *et al.* [11] for a same Rayleigh and wall emissivities to validate the results.

To do so, before launching *paraFoam*, is necessary to run the *wallHeatFlux* utility as in previous problems to generate the field of the conductive/convective heat fluxes (named *wallHeatFlux* as well). The field of the radiative heat fluxes is already present as *Qr*.

Next the user can open the case with *paraFoam*. Before clicking *Apply* he should make sure that the *Qr* and *wallHeatFlux* fields are selected in the properties menu, as well as the patch or patches of interest (and anything else), e.g. *minX*. Then an *Integrate Variables* filter can be applied which will integrate *Qr* and *wallHeatFlux* over the surface of the selected patches, therefore obtaining the global heat rates which are displayed in a table (see Figure 38). Keep in mind that they use an opposite sign criteria as *Qr* is the radiative flux entering the patch (opposite to internal face normal) and *wallHeatFlux* the flux entering the domain (same direction as the internal face normal).

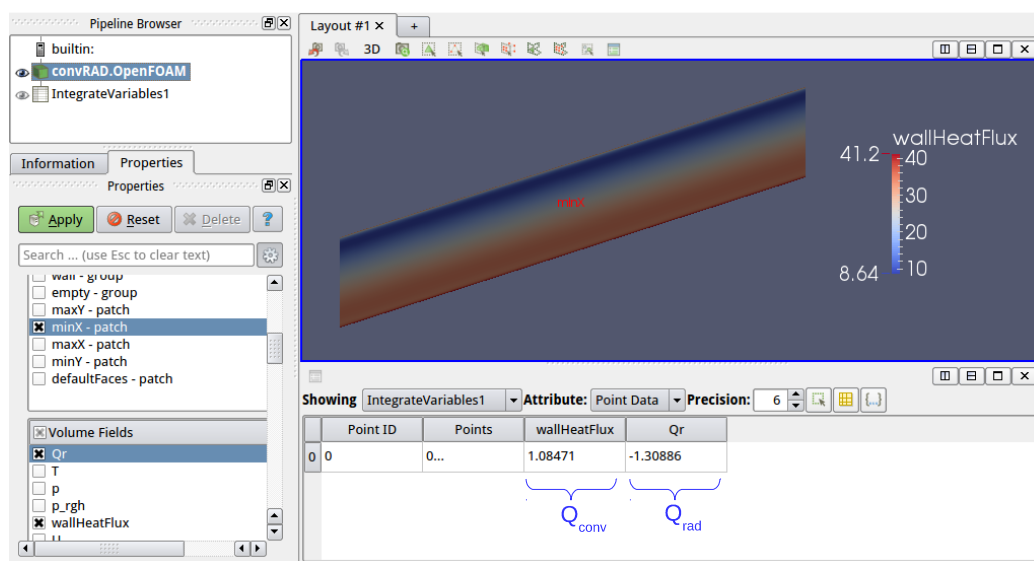


Figure 38: Using the *Integrate Variables* filter of *paraFoam* on the *minX* patch.

With this the radiative, convective and total (the sum of the two) Nusselt numbers can be calculated for the comparison with Wang's work. The results are presented in Table 11 showing a good agreement.

	This work			Wang et al.		
	$Nu_c$	$Nu_r$	$Nu_t$	$Nu_c$	$Nu_r$	$Nu_t$
Hot wall	4.211	5.081	9.292	4.189	5.196	9.385
Cold wall	4.273	5.021	9.294	4.247	5.137	9.384

Table 11: Obtained Nusselt numbers on hot and cold walls and comparison with Wang's results.

Finally the next figures show a representation of the isotherms and the streamlines. The simplest method for the representation of isosurfaces in a 2D plane is to simply reduce the *Number Of Table Values* in the *Color Map Editor* (marked in red in Figure 39).

Representation of the isotherms:

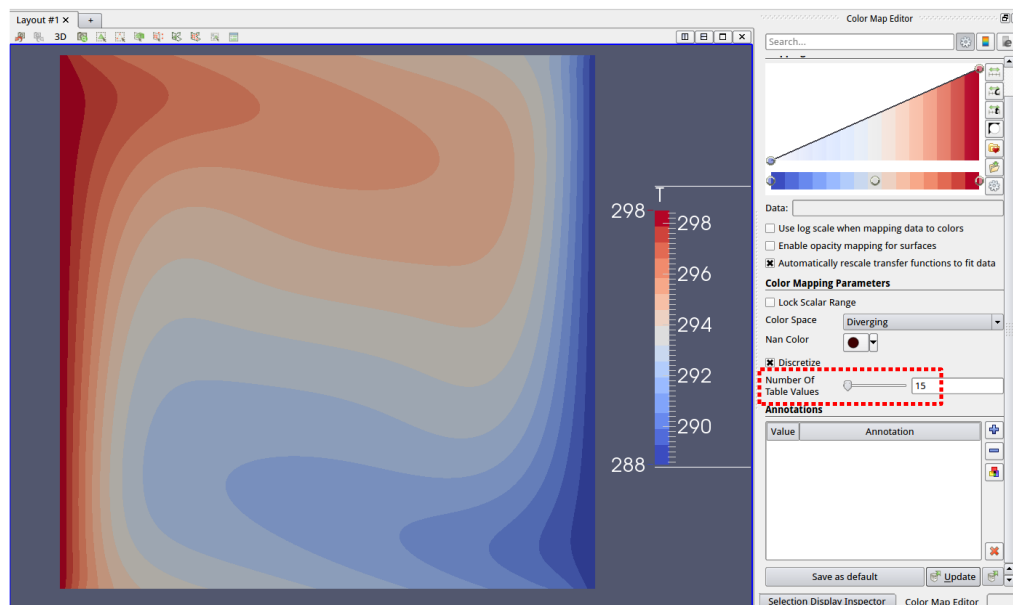


Figure 39: Isotherms.



Representation of the streamlines:

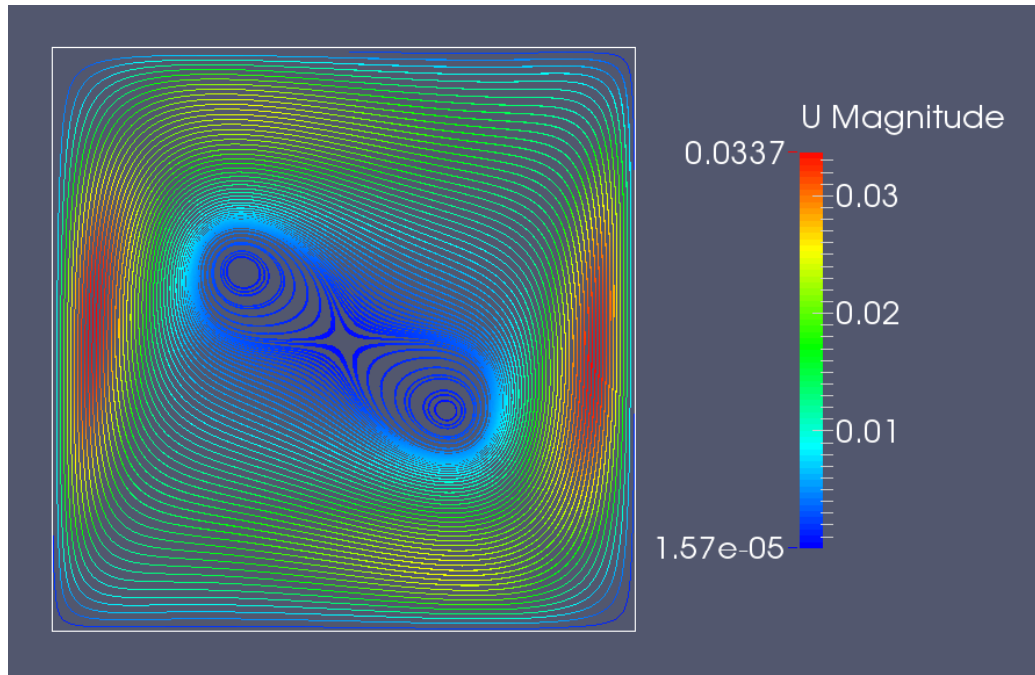


Figure 40: Streamlines.

## 5.2 Part B

### 5.2.1 Description of the problem

This case is a modification of a previous one where a heat generating solid, square block has been placed in the center (Figure 41). The heat generation is considered uniform all over the block and produces a total heat rate of 1W. The thermal conductivity of the solid material is  $\kappa = 0.5 \text{ W/(K}\cdot\text{m)}$  and the thermal emissivity is  $\varepsilon = 0.8$  on all the surfaces. The rest of parameters and properties are the same as in the previous case.

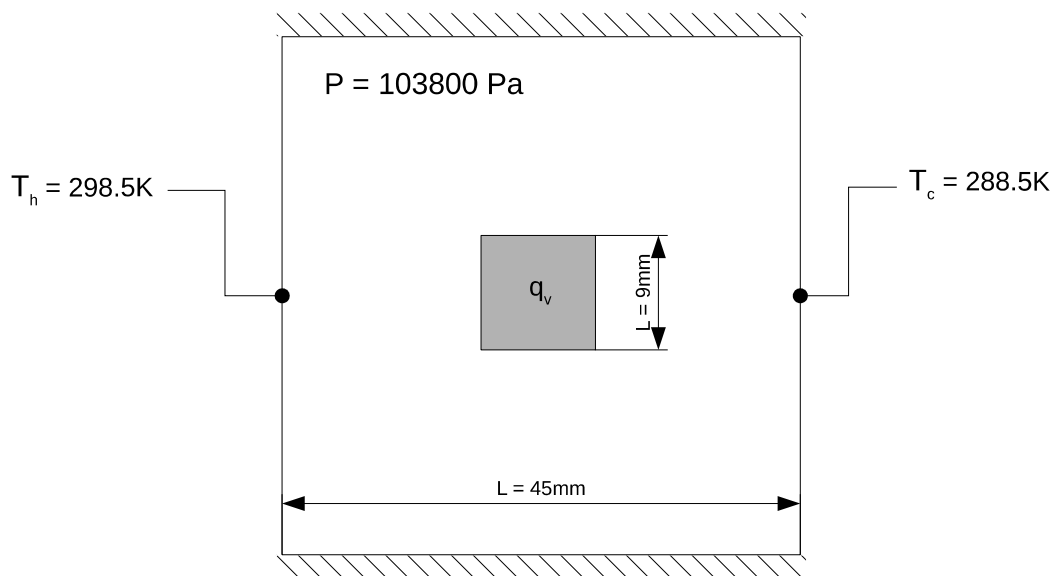


Figure 41: Diagram of the case.

#### 5.2.1.1 Assumptions

- Steady-state conditions.
- Bi-dimensional, compressible, laminar flow
- Newtonian fluid
- Perfect gas
- Constant thermo-physical properties
- Surface-to-surface radiation with non-participating medium
- All the surfaces are gray, diffuse and opaque with a constant, uniform emissivity
- Uniform heat generation inside the block

### 5.2.1.2 Formulation

The formulation relative to the air region and the radiation is the same as in the previous part, as for the solid the only change is the addition of the heat source term the the heat equation:

$$\rho c_p \frac{\partial T}{\partial t} - \kappa \nabla^2 T = q_v$$

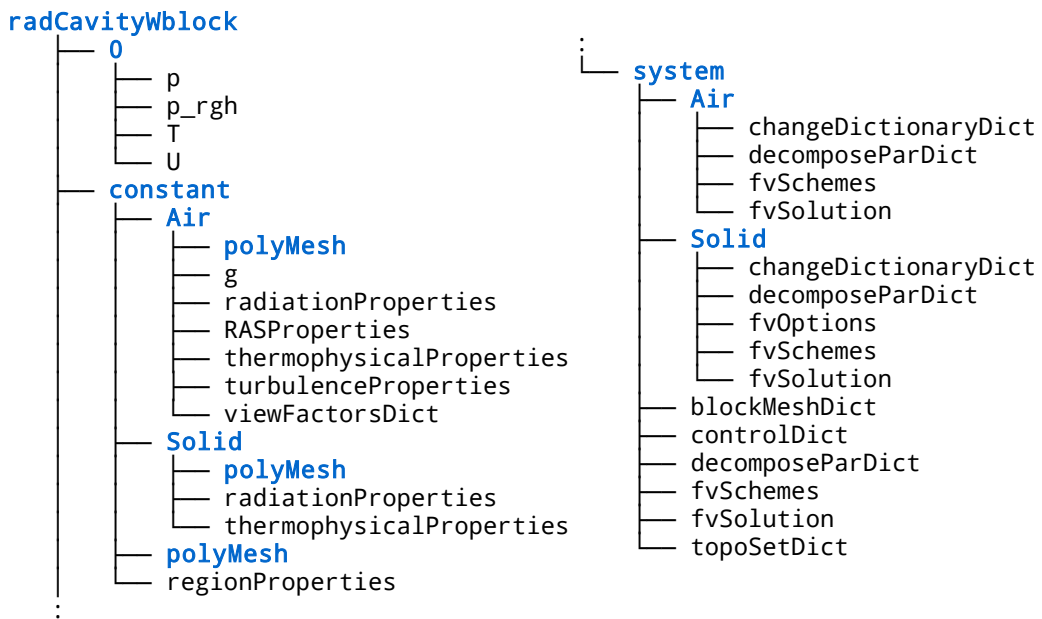
Which for a steady-state case is:

$$- \kappa \nabla^2 T = q_v$$

The `chtMultiRegionSimpleFoam` solver solves this in terms of enthalpy which will be useful to keep in mind later, when the source term is being added:

$$- \frac{\kappa}{c_p} \nabla^2 h = q_v$$

### 5.2.2 Preprocessing



This case uses the same mesh as the previous one, as well as the same external boundary conditions and the same properties for the `Air` region, therefore most of the files are the same but adapted to the file structure of the `cht solvers` which has already been detailed in previous chapters, therefore this section won't go into as much detail.

### 5.2.2.1 Boundary conditions and properties

As mentioned earlier the external boundary conditions are the same and as for the internal ones, i.e. the conditions on the patches where the two regions meet, they are introduced through the following *changeDictionaryDict* files:

/Air/changeDictionaryDict:

```

1 dictionaryReplacement
2 {
3     Qr
4     {
5         boundaryField
6         {
7             Air_to_Solid
8             {
9                 type                greyDiffusiveRadiationViewFactor;
10                emissivityMode      solidRadiation;
11                Qr                  uniform 0;
12                value                uniform 0;;
13            }
14        }
15    }
16    p_rgh
17    {
18        boundaryField
19        {
20            Air_to_Solid
21            {
22                type                fixedFluxPressure;
23                value                $internalField;
24            }
25        }
26    }
27    T
28    {
29        boundaryField
30        {
31            Air_to_Solid
32            {
33                type
34                compressible::turbulentTemperatureRadCoupledMixed;
35                Tnbr                T;
36                kappa                fluidThermo;
37                QrNbr                none;
38                Qr                  Qr;
39                kappaName            none;
40                value                $internalField;
41            }
42        }
43    }
44    U
45    {
46        boundaryField
47        {
48            Air_to_Solid
49            {
50                type                fixedValue;
51                value                uniform (0 0 0);
52            }
53        }
54    }
55 }
56 }
57
58 // *****
59
```

/Solid/changeDictionaryDict:

```

1 dictionaryReplacement
2 {
3     T
4     {
5         boundaryField
6         {
7             Solid_to_Air
8             {
9                 type
10                compressible::turbulentTemperatureRadCoupledMixed;
11                Tnbr          T;
12                kappa         solidThermo;
13                QrNbr         Qr;
14                Qr            none;
15                kappaName     none;
16                value         $internalField;
17            }
18        }
19    }
20
21 // ***** //
```

The `Qr` field for the `Air_to_Solid` patch provides an example of the `solidRadiation emissivityMode` which will get the emissivity from the `radiationProperties` file of the solid region (exposed below), but it is still possible to just specify the emissivity directly with the lookup mode.

```

1 radiation      on;
2
3 radiationModel  opaqueSolid;
4
5 absorptionEmissionModel constantAbsorptionEmission;
6
7 constantAbsorptionEmissionCoeffs
8 {
9     absorptivity      absorptivity [ 0 -1 0 0 0 0 0 ] 0.8;
10    emissivity         emissivity [ 0 -1 0 0 0 0 0 ] 0.8;
11    E                  E [ 1 -1 -3 0 0 0 0 ] 0;
12 }
13
14 scatterModel      none;
15
16 sootModel         none;
17
18 // ***** //
```

### 5.2.2.2 Adding the source term

The addition of the source term for the heat generation is done through the **fvOptions** file inside the `/system/Solid` directory. `fvOptions` is a flexible framework that allows the user to add different types of sources or constraints to the governing equations. This section explains the `scalarSemiImplicitSource` type which permits the addition of any source term of the kind  $S(X) = S_u + S_p X$

In order to make sure `fvOptions` is being properly used first is necessary to understand how OpenFOAM implements the governing equations, looking at the source code files can provide some clues on that (`/openfoam240/applications/solvers/heatTransfer/`

*chtMultiRegionFoam/solid/solveSolid.H*).

As commented in 5.2.1.2 the cMRSF solver solves the heat equation in terms of enthalpy so when using the *SemiImplicitSource* the equation becomes:

$$-\frac{\kappa}{c_p} \nabla^2 h = S(h) = S_u + S_p h$$

Hence:

$$S_u + S_p h = q_v \rightarrow S_u = q_v, S_p = 0$$

The corresponding *fvOptions* file will be:

```

1      HeatSource
2      {
3          type                scalarSemiImplicitSource;
4          active              true;
5          selectionMode       all;
6          //cellZone          cellZoneName;
7
8          scalarSemiImplicitSourceCoeffs
9          {
10             volumeMode       absolute; //alt. specific
11             injectionRateSuSp
12             {
13                 h (1 0);
14             }
15         }
16     }
17
18 // ***** //
```

*fvOptions* needs a definition of the region where the source term is applied, since in this case this is the whole *Solid* region it's only necessary to set the *selectionMode* to *all*. Another useful *selectionMode* is the *cellZone* one, with this the region is defined through a *cellZone* created with *topoSet* whose name is indicated below after a *cellZone* keyword (exemplified in line 6).

*volumeMode* allows the user to set whether the source is indicated as an absolute quantity (*absolute*) or a quantity per unit of volume (*specific*).

Finally within *injectionRateSuSp* the  $S_u$  and  $S_p$  coefficients are indicated after the name of the field of the corresponding equation (*h*). In this case since the absolute mode is used this means  $S_u = q_v \cdot V = 1 \text{ W}$  (so there's no need to care about the volume).

### 5.2.3 Running the case in parallel

As in Chapter 4 a script like this can be used to run the post-processing utilities:

```
1  #!/bin/bash
2
3  blockMesh
4  topoSet
5  splitMeshRegions -cellZones -overwrite
6
7  rm ./0/Solid/{p_rgh,U,Qr}
8
9  for i in Air Solid
10 do
11     changeDictionary -region $i > log.changeDictionary.$i 2>&1
12 done
```

And this one to begin the simulation. Notice the `faceAgglomerate` and `viewFactorsGen` need additional arguments for a multi-region case.

```
1  #!/bin/sh
2
3  decomposePar -force -allRegions
4  mpirun -np 4 faceAgglomerate -region Air -parallel -dict
   constant/viewFactorsDict
5  mpirun -np 4 viewFactorsGen -region Air -parallel
6  foamJob -screen -parallel chtMultiRegionSimpleFoam
```

### 5.2.4 Post-processing

The `controlDict` was set to run for 8500 iterations and the following results were obtained.

Global heat rates:

Patch (region)	Heat rate [W]		
	Conv./Cond.	Radiation	Total
Solid_to_Air (Solid)	-1.000	/	-1.000
Air_to_Solid (Air)	0.5098	0.4902	1.000
MinX (Air)	0.7688	0.9307	1.700
MaxX (Air)	-1.370	-1.331	-2.701

Table 12: Heat rates through different patches. Positive values for entering heat.

Isotherms:

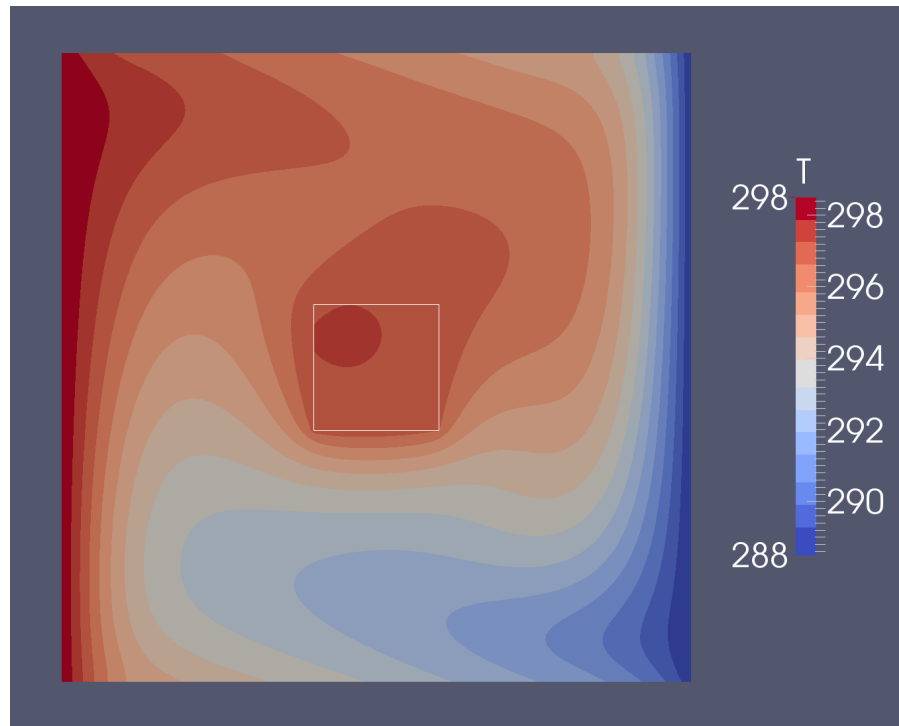


Figure 42: Isotherms.

Streamlines:

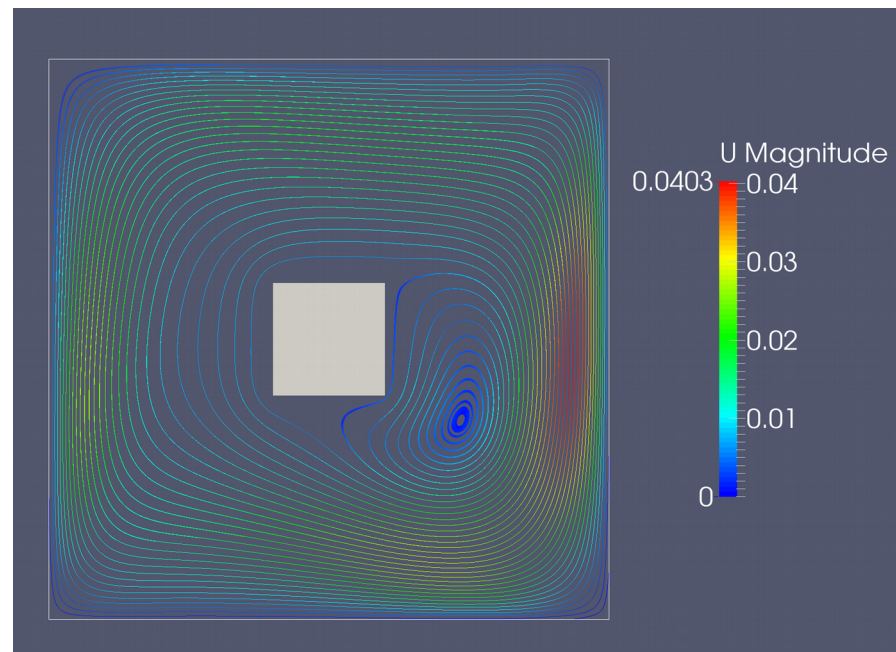


Figure 43: Streamlines.



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## Environmental impact

The realization of this project didn't produce any direct residual. The associated environmental impact is assessed as the estimated carbon footprint due to the electrical consumption during the 325 hours of work assuming an emission of 0.302g CO<sub>2</sub>/kWh [18]. The result is presented in Table 13.

It's worth to note since all the work and computation has been done with a personal computer the carbon footprint is not different than that of a typical office worker.

Average power consumption	Total energy consumption	Total CO <sub>2</sub> emissions
75 W	24.38 kWh	7.36 Kg

Table 13: Carbon footprint.

## Conclusions

The realization of the guide has achieved:

- The proposition and description of a total of eight model problems involving conduction, laminar convection and radiation phenomena.
- A complete description about the implementation of these cases using the OpenFOAM software.
- The numerical resolution of the cases using serial and parallel processing.
- A description of the main post-processing features to analyze the solution data of heat and mass transfer problems.
- The direct comparison and validation of the results of 4 of the cases and the verification of the convergence and physical consistency of the other 4.

With this project it has been found that OpenFOAM:

- Is a very versatile CFD software which can deal with a wide variety of heat and mass transfer problems.
- Is distributed under a free GPL license which can reduce the final costs significantly.
- Comes with a variety of tools to help with the mesh generation, the handling of the results and other processes.
- Is prepared for parallel processing, reducing the computation times if multiple

processors are available.

- Is not an intuitive software. The data entry is generally handled with data dictionaries and the utilities are executed through commands.
- Provides reliable results, provided the case is properly modeled.

Furthermore, as a personal conclusion, the research work for the elaboration of the guide has brought me a lot of new knowledge about OpenFOAM, which I consider very valuable as it has direct practical applications in the field of engineering; and the elaboration itself further contributed to my self-development helping me better establish both the newly acquired and the some of previous knowledge.

## Further work

Further lines of work after this project could be the:

- Deeper description of the presented meshing utilities, particularly *snappyHexMesh*.
- Study of the main numerical schemes and algorithms.
- Detailed analysis and description of the P1 and fvDOM radiation models. Use on advanced radiation problems with participating media.
- Modeling of the turbulence. Description of the principal models, range of applicability and considerations, application in thermal problems, comparison with experimental or DNS data...
- Simulation of multi-phase flows with phase-change heat transfer.
- Combustion modeling. This may require the inclusion of the previous phenomena.

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